IV. Science and Technology Strategic Plan

This chapter provides an overview of Argonne's strategic plan for research in science and technology. For Laboratory program areas, the chapter presents summary plans that describe strategies for accomplishing each program's objectives in the context of relevant issues and obstacles to be overcome.

Overall coordination of the Laboratory's planning with that of the Department of Energy takes advantage of key DOE planning documents — including the Department's overall strategic plan — that are being reformulated in 2002 to reflect current opportunities and priorities. Key documents available in early 2002 include the following:

- The national energy policy of the Bush administration, May 2001, a first step toward a comprehensive, long-term national strategy that uses leading-edge technology to produce an integrated national energy, environmental, and economic policy (URL: www.energy.gov/HQPress/releases01/maypr/energy_policy.htm).
- The annual budget request submitted by DOE to Congress (URL: www.cfo.doe.gov/budget/03budget/index.htm), including budget justifications for the Office of Science (URL: www.mbe.doe.gov/budget/03budget/content/science/sciexuc.pdf) and other DOE offices that support Argonne research.
- The *Strategic Plan* of the National Nuclear Security Administration.

Cooperation among the DOE laboratories, particularly through direct R&D collaborations, is increasingly extensive. This trend toward a more integrated laboratory system is described from an Argonne perspective in the Appendix.

A. R&D Area Strategic Plans

The balance of this chapter presents summaries of strategic plans for each of 19 planning units that span the Laboratory's major mission areas (see the inset box on the next page). These strategic plan summaries are grouped into (1) fundamental science and national research facilities, (2) energy and environmental technologies, and (3) national security. This grouping encompasses DOE's four mission areas. In addition, a concluding summary plan addresses the crosscutting topic of collaborative R&D partnerships.

The planning areas for fundamental science and national research facilities correspond closely with Argonne's scientific divisions. In contrast, Argonne's technology programs cut across Laboratory divisions to exploit multidisciplinary capabilities. (See the Argonne organization chart at the end of this volume.)

A number of the R&D area plans that follow include discussions of program-specific initiatives. These discussions complement presentation of Argonne's major Laboratory initiatives in Chapter III.

1. Fundamental Science and National Research Facilities

Argonne's activities in the area of fundamental science and national research facilities are supported predominantly by DOE's Office of Science.

a. Advanced Photon Source

Situation

The Advanced Photon Source (APS) is Argonne's premier user research facility. Its ongoing successful operation is central to the Laboratory's outstanding performance in science and technology. Built and operated for DOE-Basic Energy Sciences (DOE-BES), the APS is delivering on its promise to serve the scientific community and to enhance U.S. productivity in a broad spectrum of scientific and technological areas. Over 4,800 individuals have qualified for

Argonne's Strategic Plans

1. **Fundamental Science and National Research Facilities**
   a. Advanced Photon Source
   b. Materials Science
   c. Chemical Sciences
   d. Nuclear Physics and the Argonne Tandem-Linac Accelerator System
   e. High Energy Physics
   f. Mathematics, Computing, and Information Sciences
   g. Intense Pulsed Neutron Source
   h. Biosciences
   i. Environmental Research
   j. Science and Engineering Education and University Programs
2. **Energy and Environmental Technologies**
   a. Advanced Nuclear Technology
   b. Energy and Industrial Technologies
   c. Transportation Technologies
   d. Environmental Treatment Technologies
   e. Energy and Environmental Systems
   f. Biotechnology
3. **National Security**
   a. Nuclear Nonproliferation and Arms Control
   b. Infrastructure Assurance and Counterterrorism
4. **Collaborative R&D Partnerships**

badges to use the facility, and in 2001 nearly 500 publications were based on work performed there. International competition in this research area comes primarily from two similar synchrotron radiation centers, the European Synchrotron Radiation Facility in France and SPring-8 in Japan.

The APS began operating in 1996 as a user facility serving the worldwide community of x-ray researchers. Between 1989 and 1996, DOE invested $812 million in construction of the APS and in R&D supporting construction. The resulting world-class photon source today provides the brightest x-ray beams available in the Western Hemisphere, for a wide range of research fields such as materials science, structural biology, environmental studies, and applied engineering. Collaborative access teams — composed of investigators from private industry, universities, government, and other institutions — have committed an additional quarter billion dollars in capital investments for construction of APS beamlines. As of the summer of 2002, 28 of 34 available sectors have been assigned to collaborative access teams (CATs). (A sector comprises one bending magnet beamline and one insertion device beamline.) Included in these 28 sectors are 7 managed by Argonne staff: the Structural Biology Center (SBC) CAT, which comprises one sector; the Basic Energy Sciences Synchrotron Radiation Center (BESSRC) CAT, which comprises two sectors; and the Synchrotron Radiation Instrumentation (SRI) CAT, which comprises four sectors.

The SBC CAT is a national user facility for the study of macromolecular crystallography. It is funded through Argonne's Biosciences Division by DOE's Office of Biological and Environmental Research (DOE-BER). Designed for rapid throughput, SBC CAT provides users with the ability to collect data by employing standard crystallographic techniques and multiple energy anomalous dispersion phasing techniques.

The BESSRC CAT is a joint venture of Argonne's Chemistry and Materials Science Divisions, in partnership with the Geosciences program of DOE-Basic Energy Sciences (DOE-BES) and with Northern Illinois University. The two sectors of BESSRC CAT have been developed and instrumented for researchers in materials science, chemical science, atomic physics, solid state physics, and geosciences. Currently under development are plans for a dedicated small-angle scattering beamline and conversion of both insertion devices for use of tandem undulators. The center's existing high energy capabilities and its planned dedicated small-angle scattering facility will play important roles in the Center for Nanoscale Materials (CNM). (See Section III.A.1.)

The SRI CAT, supported through APS facility funding, focuses on developing instrumentation and techniques that utilize the unique properties of APS radiation to advance the frontiers of scientific research capabilities. Among the instruments and capabilities that have already been developed are microbeam techniques, nuclear resonant spectroscopy, high-resolution inelastic x-ray scattering, coherence-based techniques, application of high energy x-rays, and generation and use of polarized x-rays. Microbeam techniques developed at the SRI CAT will provide an important foundation for the Nano CAT, which will be associated with the CNM. (See Section III.A.1.)

The APS provides users with 5,000 hours of beam time each year. During 2001, two major enhancements were implemented in the storage ring: top-up operation and reduced emittance. Top-up operation makes APS the only synchrotron facility in the world that operates in a constant-current configuration, which delivers to users an increased number of ampere-hours and also facilitates beam stability because of the constancy of the power loading on the storage ring and optical components. Reduced particle beam emittance translates directly into higher x-ray beam brilliance. Top-up operation and reduced emittance promise to increase the productivity of APS users substantially.

Vision

The APS will function in a highly reliable manner and will remain the preeminent source of hard x-rays for the U.S. research community into the foreseeable future, serving a wide range of frontier science and technology and addressing questions of importance both nationally and internationally. To maintain its preeminence and to continue highly reliable operation of accelerator and beamline systems, the APS will implement innovative accelerator enhancements that improve beam characteristics and state-of-the-art R&D that improves experimental capabilities. Through productive partnerships with its users, the APS will focus on opportunities to serve all its customers better, thereby creating a rewarding and enriching R&D environment and enhancing the facility's worldwide leadership role.

Mission

The mission of the APS includes the following three major elements:

- Delivery of world-class science and technology through operation of a state-of-the-art synchrotron radiation facility.
- Optimization of operational reliability, availability, beam quality, and scheduled operating time to achieve excellence in serving all research users.
- Development of leading-edge accelerator and experimental technologies that advance the research capabilities of investigators from across the United States and around the world.

Goals and Objectives

The overall goals of the APS are (1) to increase beam availability, beam quality, and scheduled operating time for both insertion devices and bending magnet sources and (2) to provide the technical and administrative support needed to maximize researcher productivity.

Major objectives are as follows:

- Maintain accelerator operations at better than 95% availability in 2003.
- Maintain operating time scheduled for users at 5,000 hours for 2003.
- Enhance the research capabilities available to users.
- Ensure accessibility of the facility to a broad spectrum of users.
- Provide essential services to APS users in the areas of technical support, operations, safety, administration, and general services.
- Optimize the scientific and technological benefits to society from research at the APS.

In all these endeavors, highest priority is given to ensuring the health and safety of employees, users, and visitors and to protecting the environment.

Issues and Strategies

The APS is currently processing applications from two prospective CATs planning research in the field of structural biology, more specifically in macromolecular crystallography. Agreements with both CATs are expected in 2002. The CATs will be assigned the last two spaces available in the just completed laboratory/office module (LOM) 436, which was funded by the National Institutes of Health and DOE-Biological and Environmental Research.

Five additional prospective CATs are in various stages of writing proposals and raising funds: (1) Nano CAT, (2) Inelastic X-ray Scattering (ISX) CAT, (3) Midwest Center for Structural Genomics (MCSG) CAT, (4) Environmental (Enviro) CAT, and (5) the High Energy X-ray (HEX) CAT. Argonne staff members are playing leadership roles for all five of these prospective CATs. The missions of the five prospective CATs are as follows:

- Nano CAT will be associated with the CNM (see Section III.A.1). Nano CAT will provide the CNM with capabilities to characterize and study nanostructures through a variety of techniques.
- ISX CAT, a partnership among several national laboratories and universities, will be optimized for inelastic x-ray scattering at the APS. It will provide researchers with capabilities unique in the Western Hemisphere.
- MCSG CAT will be a high-throughput macromolecular crystallography beamline associated with the Midwest Center for Structural Genomics. It will focus on biostructures as they relate to structural genomics. (See Section IV.A.1.h.)
- EnviroCAT will provide beamlines dedicated to a wide variety of techniques valuable for environmental studies. Institutional members of the CAT include national laboratories and universities. (See Section IV.A.1.i.)
- HEX CAT is envisioned as a sector optimized for the use of high-energy x-rays, very penetrating radiation with a variety of applications to both basic and applied science. The capabilities of HEX CAT will complement those of Argonne's Intense Pulsed Neutron Source (IPNS). (See Section IV.A.1.g.)

Approval of these CATs is expected within the next few years, which will leave only one APS sector uncommitted and available to serve new research programs. Two of the prospective CATs (Nano and MCSG) are associated with facilities proposed as part of major Laboratory initiatives. Buildings for both facilities, to be located in close proximity to the APS, will provide laboratory and office support for the associated CATs. However, no LOM exists to support the remaining prospective CATs. Funding is needed for the final LOM, to support sectors 27, 28, 29, and 30, so that the building will be available when it is needed by the CATs. Additional funding will also be needed to upgrade building services (e.g., heating and cooling) for new CATs.

The APS is a high-quality research facility with excellent, experienced staff. Although all the technical design parameters of its accelerator systems have been achieved, the facility's accelerator physics staff continues to focus on responding to ever-increasing user demands for the best possible operational reliability and availability. To remain at the scientific forefront and to maintain the excellence of its in-house research staff, the APS must continue to develop and meet technically challenging research objectives in accelerator physics, insertion device development, beamline design, optics R&D, and other areas. Beyond these technical challenges, APS currently faces the new administrative challenge of supporting operation of CATs funded by DOE-BES. The Laboratory is evaluating how best to balance this challenge with the need to maximize scientific productivity while maintaining the world-class in-house staff required to maintain the leadership role of the APS. Additional annual resources of approximately $1.5 million per sector on average will be needed for the APS to assume responsibility for the BES-funded CATs.

Initiative: Enhancement of the APS and Development of Future Light Sources

Over the past three decades, the brilliance of x-ray sources has doubled every ten months. Use of coherent flux, which is directly proportional to beam brilliance, has had major unforeseen benefits for research in life sciences, soft condensed matter, and materials science, even though the flux values currently available at the APS are relatively low. To achieve the benefits expected from future experiments at higher brilliance, it is imperative that planning begin now for a 10- to 100-fold increase in APS beam brilliance by 2006 (the tenth anniversary of facility operations). Such an increase in beam brilliance will require upgrading the storage ring and insertion devices. Maximizing gains in research productivity from the increased beam brilliance also requires improved beamlines, optics, and detectors.

To increase beam brilliance, R&D is needed on paths to higher currents, on techniques for further reducing particle beam emittance, on lengthening straight sections in the storage ring, and on upgrading insertion devices to better match future operational parameters of the storage ring, as well as on other problems. Upgrading an insertion device involves optimizing it for the particular scientific mission of a beamline, which requires R&D on undulator period optimization, on more extensive use of small-gap vacuum chambers, on in-vacuum and superconducting undulators, on development of nonplanar (figure-eight) devices, and on long insertion devices (for longer straight sections). Also required is aggressive study of how to tailor the storage ring parameters (i.e., beta functions, canted undulators, and straight-section lengths) for particular beamlines.

Design of many current APS beamlines began over a decade ago, and some already need upgraded components. Greater x-ray beam brilliance will heighten the need to upgrade beamlines. For example, mirror quality has improved enormously since the first beamline mirrors were ordered, and most of the mirrors currently installed will not be able to deliver to the sample a beam brilliance increased by two orders of magnitude. Other optical components will be similarly inadequate. Detector development is perhaps most urgent, and in many cases it is already on the critical path to faster data collection.

Now on the drawing board are what can well be called the second generation of beamlines for the APS. These highly specialized beamlines are being designed so that their radiation properties optimize a particular type of research, such as inelastic x-ray scattering, high-energy x-ray scattering, or nanoprobe applications. Development of the second-generation APS beamlines presents new challenges to beamline scientists and engineers, and support for their efforts is needed if the APS is to remain at the forefront of scientific research.

Long-range plans are also being developed for other improvements to the APS storage ring that will enable it to lead the way into the next decade of x-ray science and technology. Argonne is developing concepts for further reducing the particle beam emittance by (1) operating the APS at a lower stored beam energy, (2) reconfiguring the magnetic lattice, or (3) using the existing booster and storage ring as the primary components of an energy recovery linac system to achieve a diffraction-limited, femtosecond x-ray source. Novel concepts such as these would create APS capabilities that are qualitatively and quantitatively different, and considerable R&D will be required to verify their feasibility.

In the late 1990s the Basic Energy Sciences Advisory Committee (BESAC) gave first priority to R&D on sources exploiting an 8- to 20-keV x-ray laser. Argonne has joined five partners — Brookhaven, Los Alamos, and Lawrence Livermore National Laboratories; the Stanford Linear Accelerator Center (SLAC); and the University of California at Los Angeles — to develop a proposal for a laser in the required wavelength range. Development of the proposed facility, the Linac Coherent Light Source (LCLS), will make use of the two-mile linear accelerator at SLAC and will take advantage of the distinctive capabilities of each of the partner institutions. Argonne has agreed to develop the integrated undulator systems for the LCLS. This work, which will account for about 20% of the total estimated project cost, will be funded separately from APS operations.

The original LCLS Scientific Advisory Committee, led by Gopal Shenoy (of Argonne) and Joachim Stohr (of Stanford University), gave BESAC a detailed proposal for pioneering experiments in atomic, molecular, plasma, and laser physics; in protein crystallography; and in nanoscale dynamics in condensed matter. Argonne researchers must start now to develop the optics, instrumentation, beamlines, and experimental techniques for the next generation of laser-based x-ray experiments if they are to lead the use of the

LCLS and remain at the forefront of synchrotron radiation research. For example, this unique facility will undoubtedly have major scientific impact in areas such as femtosecond time-resolved studies. The expertise needed for such studies should be developed now, so high priority should be given to a strong program of pump-probe studies using the APS with its current characteristics. Time-resolved studies, currently under way at the APS though in a nascent stage, should be expanded in scope and enhanced to improve temporal resolution, in order to fully exploit the unique science achievable through this largely unexplored field of study.

To begin exploring the physics and scientific applications of free electron lasers (FELs), the APS is examining the possibility of organizing the FEL CAT. Unlike other synchrotron-based facilities, FEL CAT would not use x-rays generated by charged particles in the synchrotron storage ring. Rather, it would use ultraviolet radiation generated by the low-energy undulator test line (LEUTL). Today no tunable laser systems of any sort operate in the wavelength range, below roughly 150 nanometers, that would be accessible to the proposed system. This very interesting wavelength range is today virtually unexplored by any tunable, high-power, pulsed laser system anywhere in the world.

Required resources are described in Table IV.1. Funding will be sought from DOE-BES (KC).

Table IV.1 Enhancement of the APS and Development of Future Light Sources
($ in millions BA, personnel in FTE)

	FY03	FY04	FY05	FY06	FY07	FY08	FY09	FY10
Costs								
Operating	0.5	1.0	2.0	2.5	3.0	3.8	4.0	4.2
Capital Equipment	0.5	5.0	7.0	12.0	12.0	8.0	6.0	3.0
Construction	-	-	-	-	-	-	-	-
Total	1.0	6.0	9.0	14.5	15.0	11.8	10.0	7.2
Direct Personnel	2.0	5.0	7.0	9.0	11.0	13.0	15.0	15.0

b. Materials Science

Situation

Research in materials science at Argonne addresses critical issues underlying the development of new and improved materials that play crucial roles in both the national economy and DOE mission areas. The Laboratory's work embraces experimental and theoretical studies, as well as computer simulations. Argonne programs provide the fundamental understanding of novel materials that will underpin tomorrow's technologies. These programs emphasize the broad scale and depth of investigation that are possible within the national laboratories.

Argonne's user facilities for materials research feature prominently in Laboratory research programs. The Laboratory plays a leading role in developing the instrumentation and experimental design needed to apply its facilities to problems at the frontiers of materials science. Argonne programs stress collaboration with leading scientists at the Laboratory, across the nation, and around the world.

Key materials research areas at Argonne include superconductivity, magnetism, ferroelectricity, ceramic films, metals, carbon, biomaterials, and nanoscale materials science and technology. Crosscutting research themes are emphasized, especially complex oxides, interfaces, and defect production.

Vision

Argonne will foster world-class materials science, forefront instrumentation, and unique user facilities. The combination of individual freedom and teamwork that nurtured past successes will be strengthened. The Laboratory's contributions to new materials, especially at the nanoscale, will support both DOE and the nation in meeting new scientific, technological, and economic goals.

Objectives

Specific objectives of Argonne's research are as follows:

- Develop forefront programs in nanoscale materials science that explore the effects of confinement, proximity, and organization in magnets, superconductors, and ferroelectrics.
- Develop and apply innovative neutron scattering science to the investigation of materials, in preparation for the advent of the Spallation Neutron Source.
- Understand and exploit the rich diversity of behavior in complex materials, including oxides, polymers, biosynthetic composites, and carbon.
- Develop novel instrumentation that drives the frontier of science at the APS and the Electron Microscopy Center (EMC).

Issues and Strategies

Today is a time of high opportunity in condensed matter and materials physics. National attention on nanoscience has revealed new horizons for creating, understanding, and controlling novel behavior in materials arising from their nanoscale structure. Now within reach are grand challenges in materials fabrication by lithography and self-assembly, as well as in materials characterization using scanning probe microscopy, electron microscopy, focused x-ray scattering, and neutron scattering. Moreover, a complementary national emphasis on biology and medicine reveals many opportunities for adapting the traditional tools and ideas of materials physics to the study of genomes, proteins, and living cells. Qualitatively new materials and functionality can be created at the "hard-soft" interface between biology and condensed matter. All these directions are part of a general trend in materials physics toward increasing complexity. Exploiting this rich diversity of behavior will require new concepts and new approaches to integrating interdisciplinary experiments and theory in a comprehensive research program.

Argonne will take advantage of these unusual opportunities to strengthen its contributions to materials science. Creation of a new CNM (see Section III.A.1) will extend the Laboratory's reach in materials science through development of fabrication facilities, a nanoprobe x-ray beamline at the APS, and new nanoscale characterization instruments. With other national laboratories, Argonne is developing a National Transmission Electron Achromatic Microscope (NTEAM) that will bring subnanometer spatial resolution and real-time response to a host of new materials experiments. The Laboratory is launching new programs in biosynthetic materials and spin-electronic materials and is teaming with other national laboratories to develop Centers of Excellence in Synthesis and Processing, in the areas of granular materials, permanent magnetism, ultrananocrystalline diamond, and ferroelectrics.

Argonne emphasizes excellent basic science as the cornerstone of its materials science program. The Laboratory continuously refreshes its program mix by adding new directions as new materials are discovered and research capabilities grow. Argonne stresses comprehensive programs that incorporate integrated experimental and theoretical thrusts and exploit advanced scientific instrumentation ranging from benchtop scanning probes to unique x-ray and neutron sources. The Laboratory regularly attracts outstanding international scientists as collaborators in its interdisciplinary programs. Leading theorists are attracted to the new Materials Theory Institute for stays of one week to six months that support key experimental programs. The resulting extensive professional network is invaluable as a source of intellectual stimulation and also as a source of outstanding candidates for postdoctoral and permanent positions.

Two important new directions in Argonne's materials science program are nanostructured biocomposite materials for energy transduction and spin-polarized oxides.

Argonne has launched an interdisciplinary program for the design, synthesis, and characterization of a new class of nanostructured biocomposite materials that exploit the capabilities of biological molecules to store and transduce energy. The goal is to organize complex biological molecules (e.g., light-harvesting proteins) into artificial host structures where the biological function can be optimized and exploited. An interdisciplinary team of materials scientists, chemists, and biologists will use a novel lipid-based complex fluid and a rigid mesoporous inorganic framework as the host materials for biomolecules. This novel approach to nano-structured biomaterials that exploit biological functions has great scientific interest and enormous technological value. Research results are expected to provide fundamental insight into ways to use soft and hard materials to construct complex architectures that combine the functionality of biomolecules with the novel properties of host materials. This work will also provide fundamental knowledge of (1) nanoscale phenomena occurring at the interfaces between the integrated materials and (2) means to tailor energy transduction processes. Results could lay the groundwork for producing the next generation of materials for use in sensors, optoelectronics, artificial organs, and catalysis. This project will use major Argonne research facilities, including the APS, the IPNS, the EMC, the Advanced Computer Research Facility, and the planned CNM (see Section III.A.1). Also available for this project will be the facilities of the Center for Nanofabrication and Molecular Self-Assembly at Northwestern University. These major facilities provide unique capabilities for synthesizing and characterizing new biomaterials, as well as for understanding and tailoring their properties.

As the end of the silicon roadmap appears on the horizon, new kinds of electronics will be needed to meet the ever-increasing demands of information, energy, and national security technologies. Prominent among candidate approaches to sustaining the pace of progress is spin-electronics, or spintronics. In spintronic structures, information is stored and transmitted by using the spin of the electron, as well as its charge. Argonne contributes to fundamental understanding of materials issues affecting spin-polarized transport and develops ways of controlling and tailoring relevant materials properties. The central goal is to understand how the materials, their three-dimensional confinement into nanostructures, and their interfaces affect the generation and transmission of spin-polarized current. Pursuit of this goal will follow three parallel themes: (1) effects of confinement on phase behavior, (2) surface structure, and (3) interfaces and their impact on spin-polarized transport. This work builds on Argonne's expertise in the synthesis and measurement of naturally layered manganites by creating artificially layered manganites that generate new spin-polarized oxide nanostructures. The work will be linked strongly with the APS, the EMC, and the IPNS, which provide unique scattering tools capable of revealing the new science underlying complex magnetic materials. The resulting fundamental knowledge of spin transport in complex oxides could enable development of the next generation of memory and logic devices.

User Facility: Electron Microscopy Center

Situation

Argonne's EMC provides transmission and scanning electron microscopy for high-spatial-resolution imaging, microanalysis, and *in situ* research. The EMC includes the Intermediate Voltage Electron Microscope (IVEM)-Tandem, which is used for a variety of *in situ* studies, especially for dynamic recording and structural characterization of the effects of ion irradiation. The IVEM-Tandem is the only facility in the Americas having this specialized capability, and it is employed by the international community. Qualified users access this facility by submitting written proposals that are peer reviewed. Nonproprietary research incurs no use charges. EMC users — including researchers from universities, other national laboratories, and industry — conduct studies ranging from imaging of electron-sensitive soft materials to *in situ* observation of phenomena at elevated and cryogenic temperatures in pure metals and alloys, semiconductors, and ceramics.

Other instrumentation in the EMC includes a state-of-the-art transmission electron microscope (TEM) with field emission gun and excellent analytical capabilities. Earlier acquisition of a scanning electron microscope (SEM) with field emission gun broadened surface analytical capabilities significantly.

Vision

The EMC will develop new techniques and methods, state-of-the-art instrumentation for TEM and SEM work, and capabilities for *in situ* studies. The materials research thus supported will provide important new insights for major technologies in such areas as micromagnetics, irradiation effects in high-temperature superconductors, solid-state amorphization reactions, and analysis and control of nanostructures.

Issues and Strategies

Argonne's High Voltage Electron Microscope-Tandem Facility was decommissioned in FY 2001. The IVEM-Tandem, which retains the capability for *in situ* studies of ion beam irradiation, needs to be supported as a special national resource in materials research. Argonne is upgrading the microanalysis and image-recording capabilities of the IVEM-Tandem and has undertaken a new program to improve *in situ* experimentation based on new designs for holders and samples.

Initiative: National Transmission Electron Achromatic Microscope

Thanks to advances in aberration correction and quantitative-transmission electron microscopy, a new generation of electron microscopes can be built that are capable of sub-angstrom image resolution and sub-electron-volt spectroscopic resolution and that have space adequate for a variety of important experiments on advanced materials. To take advantage of these new technologies, Argonne has proposed the NTEAM. The required instrumental development could be carried out cooperatively at DOE's four national centers for electron beam microcharacterization, with each center contributing a complementary specialized facility based on a common platform.

The revolutionary combination of space and resolution envisioned for the NTEAM will allow the electron microscope to be converted into a true experimental materials science laboratory. Scientific impacts to be expected include the first three-dimensional atomic imaging of defect structures; the first atomic structure determination of a glass; microscopic understanding of magnetism and ferroelectricity in nanostructures; visualization of dislocation interactions in nanostructures under controlled stress; development of interface science to the level of surface science; understanding of grain boundary motion under stress in nanocrystals; understanding of chemical reactions on highly curved, small catalyst particles; and imaging of defects in the oxygen sublattice of complex oxides. More generally, advances in electron beam microcharacterization associated with the development of NTEAM will be crucial for proper implementation of the planned national thrust in nanotechnology. The NTEAM project would also help to revitalize the critically important electron optics industry in the United States.

Following an international workshop held at Argonne in FY 2000, the Laboratory has pursued preliminary planning for an NTEAM instrument. A partnership of national laboratories is requesting permission to submit a formal proposal and is involving the research community in the planning. Seed funding from DOE is being used to advance designs for aberration-corrected microscopes. These efforts will also contribute importantly to Argonne's growing research in nanoscience.

c. Chemical Sciences

Situation

Chemistry is a core capability of the Laboratory. World-recognized research programs and staff with cutting-edge expertise study fundamental scientific questions critical to DOE's mission. Argonne research provides the foundations for addressing issues of energy independence, environmental sustainability, and national security and will underpin new technologies for energy efficiency, energy conversion, combustion, cleanup and disposal of radioactive and nonradioactive waste, and catalysis.

Vision

Argonne will enhance its status as a leading performer in chemical science research through sustained preeminence in established research focus areas and new multidisciplinary research challenges based on Laboratory core competencies.

Objectives

Specific long-range objectives of Argonne's core research in the chemical sciences are as follows:

- Advance understanding of the elementary chemical reactions and related nonreactive energy transfer processes involved in combustion by combining theoretical analysis of the energetics and dynamics of chemical reactions with experimental study of chemical dynamics and kinetics.

- Examine the chemical and physical properties of clusters of catalytically active transition metal atoms through combined experimental and theoretical studies that address, for example, how cluster properties evolve with size and how cluster chemistry depends on structure.

- Establish a refined, quantitative understanding of x-ray interactions with atoms and molecules to provide a fundamental basis for x-ray methods used in scientific investigations.

- Identify the mechanisms responsible for optimizing photochemical energy conversion in natural photosynthesis; use this information to develop artificial photochemical systems capable of enhanced photochemical energy conversion.

- Improve understanding of the initial physicochemical phenomena and molecular processes that occur when energetic radiation interacts with matter, through the use of pulsed-electron accelerators and very intense high-energy lasers causing excitation in the fastest time domains.

- Improve understanding of the interplay between f-elements and their environment through innovative experimental approaches, including laser-based methods such as (1) nonlinear laser spectroscopy, (2) optically detected nuclear magnetic resonance (NMR), and (3) *in situ* x-ray absorption fine-structure spectroelectrochemistry at the APS.

- Advance metal ion separations science by conducting fundamental investigations of the interactions of metal ions with chelating agents and solvent molecules, by designing and characterizing new reagents for more effective separations, and by examining the physical and chemical characteristics of metal ion separation processes.

- Elucidate the important molecular and physical structural features of disordered carbonaceous materials — such as soots, heavy hydrocarbons, and coals — through use of state-of-the-art tools including synchrotron x-ray spectroscopy and scattering, neutron scattering, solid-state NMR spectroscopy and imaging, and laser desorption time-of-flight mass spectrometry.

Issues and Strategies

Argonne's core research programs in chemical sciences pursue their objectives by integrating special expertise with unique research tools and facilities. Staying at the forefront depends on developing novel experimental tools.

Current strategic initiatives have established the following important new research directions:

- Study, in real time, structural changes in short-lived reaction intermediates in photochemical processes by synchronizing x-rays from the APS with a laser pulse. Recent Argonne work has shown that a heme molecular mimic undergoes a structural change after interaction with laser light.

- Study charge thermalization and transport in polar and nonpolar liquids and solids by using the recently completed tabletop terawatt laser for ultrafast pulse radiolysis.

- Monitor particle aggregation and disaggregation in real time by using the small-angle x-ray scattering instrument at the Basic Energy Sciences Synchrotron Radiation Center at the APS. A high-resolution annular detector now under construction will enable *in situ* examination of soot particle formation in flames. This new capability will also benefit other areas of investigation, including the study of dynamic protein structures.

The following recent developments will affect the direction of Argonne's core research programs in chemical sciences:

- Increased understanding of the fundamental electronic nature of bond breaking was obtained by using photoelectron spectroscopy to probe the absorption of light and redistribution of the energy throughout a molecule. Vibrational autoionization of ammonia shows a profound preference for a single mode; this mechanism is expected to be active in a broad range of molecules.
- New catalysts are being developed that can be used in "green" solvents such as supercritical carbon dioxide, in order to reduce use of volatile organic compounds.
- A large multi-investigator study led by Argonne has demonstrated that the previously accepted value of the bond dissociation energy of water needs to be modified. This result will necessitate a cascade of changes to the values of many fundamental thermodynamic parameters tabulated for species and reactions containing OH.
- Reflectivity experiments on oxygen crystal truncation rods reveal a cyclic evolution of laterally ordered water molecules on a conducting RuO_2 surface. These results are important for understanding the interfacial electrochemistry of the electrolysis processes in fuel cells.

The chemical science goals in Argonne's major Laboratory initiative Center for Nanoscale Materials (see Section III.A.1). derive directly from the Laboratory's core expertise in areas including (1) the assembly of nanostructures from gas-phase clusters or fluidic phases, focusing on understanding the forces that drive aggregation and developing experimental and theoretical methods for controlling the assembly of nanostructures; (2) controlled reactivity in hybrid nanostructures, focusing on understanding and controlling photochemical, catalytic, and biological reactivity in bioinorganic hybrids and mesoporous structures at the nanoscale (an area in which the project Nano-Engineering the Biomolecule-Inorganic Interface for Integrated Photochemistry and Catalysis has been funded); and (3) information transfer between nanodomains, focusing on understanding the principles by which the communication between nanoscale devices (sending and receiving) can be organized and controlled. Argonne's expertise in transient spectroscopies, x-ray synchrotron science, photochemistry, and theory, coupled with emerging expertise in scanning-probe microscopy, will be critical for understanding these phenomena. The Laboratory has initiated a program in nanophotonics for these studies.

Argonne's integrated program in the fundamental chemistry of radioactive waste is partly supported by the DOE Environmental Management Science Program. The Laboratory is uniquely qualified to undertake this program through its core capabilities in chemical separations science, heavy-elements chemistry, radiation chemistry, and theoretical chemistry, as well as through its facilities for research with radioactive materials (including the facility for actinide studies at the APS and the NMR facility designed for studying radioactive materials). This program of experimental and theoretical research responds to a national need for greater fundamental knowledge of the chemistry underpinning technologies for the cleanup and disposal of radioactive waste.

Argonne has developed two research programs in the chemical sciences in response to DOE's Nuclear Energy Research Initiative (NERI). One program focuses on (1) an innovative, single-material, minimum-volume approach to the selective sorption of most metal ion radionuclides from aqueous waste solutions and (2) the subsequent creation of a final nuclear waste form that is suitable for long-term storage or burial. In the other NERI research program, Argonne is studying radiation-induced corrosion relevant to the design of next-generation reactors. Higher energy efficiency can be achieved by operating pressurized-water reactors at pressures and temperatures well beyond those necessary for the formation of supercritical water. This work will consider the possibility of radiolytic water decomposition under such conditions.

Argonne is partnering with Northwestern University in the Institute for Environmental Catalysis. This partnership takes advantage of the Laboratory's expertise in magnetic resonance, pulse radiolysis, synchrotron research at the APS, and heterogeneous catalysis. In addition, Argonne is a partner with Ohio State University in a second institute that focuses on the role of environmental molecular interfaces in the chemical and biological reactivity of pollutants. This collaboration will leverage Argonne's expertise in solid-state NMR, high-field electron paramagnetic resonance, and surface science.

Argonne has a new program in computational chemistry in response to DOE's Scientific Discovery through Advanced Computing initiative. In collaboration with Sandia National Laboratories and several universities, the program focuses on software for calculating and applying reaction kinetics and dynamics. This effort exploits the Laboratory's expertise in chemical dynamics, theoretical chemistry, and computer science and is part of the multilaboratory initiative Chemical Science Discovery through Advanced Computing: A Multi-Scale Collaboration. A second part of this program will develop the foundation for statistical methods and algorithms that provide internally consistent tables of active thermodynamic values.

d. Nuclear Physics and the Argonne Tandem-Linac Accelerator System

Situation

Review committees have consistently identified Argonne as one of the world's centers of excellence in nuclear physics research. The Laboratory's leadership role in planning the Rare Isotope Accelerator, the next-generation nuclear physics accelerator, will continue this tradition. The Argonne program has many strengths, including (1) low-energy heavy-ion physics, which is largely performed at the Argonne Tandem-Linac Accelerator System (ATLAS) facility (discussed below); (2) medium-energy nuclear physics, which emphasizes the use of lepton beams (at Fermilab, TJNAF [the Thomas Jefferson National Accelerator Facility], and DESY [Deutsche Elektronen Synchrotron]) as probes into the nuclear medium; (3) the study of relativistic heavy-ion collision dynamics by using beams from Brookhaven's newly commissioned RHIC (Relativistic Heavy Ion Collider); and (4) nuclear theory, which focuses on developing fundamental understanding of hadronic and nuclear structure, reactions, and dynamics.

Vision

Argonne's nuclear physics program will resolve fundamental questions concerning the characteristics and dynamics of nuclear and subnuclear degrees of freedom in nuclei and nuclear matter. This work will involve continuous development of more powerful research apparatus and methods and the use of unique research facilities at Argonne and throughout the world.

Objectives, Issues, and Strategies

Argonne's work in low-energy heavy-ion physics will take full advantage of the unique capabilities of ATLAS to explore and understand nuclei at the limits of their stability: at high excitation energies, in exotic shapes, at rapid rotation, and with extreme proton-to-neutron ratios. Producing and detecting previously unknown isotopes and studying their structures can benefit greatly from secondary (radioactive) beams, which can provide access to regions of nuclei not currently accessible with stable beams. This approach will also allow laboratory study of key reactions in astrophysics and in the creation of the elements — reactions that occur in astrophysical settings and involve short-lived nuclei. To this end, Argonne is proposing a national Rare Isotope Accelerator that will be based largely on novel superconducting accelerator technology originally developed at the Laboratory and used for ATLAS. (See Section III.A.2.)

Argonne's work in medium-energy nuclear physics uses energetic lepton beams to increase understanding of quark and meson degrees of freedom in nuclei and the role of the quark-gluon structure of nucleons in shaping the character of nuclear forces. Laboratory researchers are playing a leading role in the research program at TJNAF, emphasizing the use of a general-purpose magnetic spectrometer constructed at the facility by the Argonne group. At DESY the Argonne group emphasizes use of a dual-radiator ring-imaging Cerenkov detector in the Hermes experiment to study the spin structure of the proton. In addition, the Laboratory is developing new technologies in laser atom trapping of noble gas atoms for sensitive trace isotope analyses and for tests of fundamental symmetries.

Argonne's work in nuclear theory addresses the dynamics, structure, and reactions of (1) quark and gluon degrees of freedom in hadrons and (2) meson, nucleon, and nucleon resonance degrees of freedom in nuclei and nuclear matter. Using Argonne's massively parallel IBM and Chiba City computer systems and the National Energy Research Scientific Computing Center IBM SP, the Laboratory's nuclear theory group has set world standards for calculations of nuclear many-body problems in which it addresses fundamental questions in nuclear structure and nuclear astrophysics. The Argonne theory program provides important guidance for current and future experimental programs at ATLAS, TJNAF, and RHIC.

User Facility: Argonne Tandem-Linac Accelerator System

Situation

ATLAS is a DOE-designated national accelerator facility for research in nuclear physics that employs beams of low-energy heavy ions. The accelerator provides high-quality beams of all the stable elements up to the heaviest, uranium. A recently completed electron cyclotron resonance ion source has increased beam intensity by an order of magnitude. ATLAS is based on a technology developed at Argonne that employs superconducting radio frequency accelerator cavities. The ATLAS facility serves a broad community of about 300 users from more than 40 research organizations and universities.

Vision

The ATLAS facility will operate reliably and provide its national community of users with unique heavy-ion beams for research at the forefront of nuclear, atomic, and applied physics. Argonne will collaborate with U.S. industry to search for new applications of the superconducting radio frequency technology pioneered for ATLAS.

Objectives, Issues, and Strategies

The ATLAS program continues to optimize its operations and develop new linear accelerator technology to provide beams of higher intensity with excellent phase space and fast timing. Operational issues are reviewed continuously, and the facility's capabilities are frequently enhanced. Argonne will be investigating technical and research issues relating to acceleration of beams of short-lived nuclei, as a basis for proposing development of a Rare Isotope Accelerator based on ATLAS. (See Section III.A.2.)

e. High Energy Physics

Situation

Argonne performs cutting-edge research on the physics of elementary particles and develops the instruments and accelerators needed to make that physics accessible. This work in high energy physics leverages a range of diverse resources that generally are available only at a national laboratory. Argonne's program includes five experiments at different stages of preparation or data taking, a varied theoretical program, and R&D on advanced methods of particle acceleration potentially suitable for future research facilities.

Argonne researchers perform experiments at high energy accelerator facilities in the United States and Europe. Other experiments are performed in special laboratory facilities without accelerators. In all projects, special attention is given to collaboration with university groups. This collaboration encompasses joint work on detectors and detector subsystems, as well as support for students working on theses in association with Argonne staff members.

Vision

To deepen and extend understanding of the physics of elementary particles, Argonne will provide scientific leadership and will design and assemble major components of the required experimental systems. The Laboratory will choose studies in theoretical physics for relevance to the Argonne's experimental program or for general potential to advance understanding of interactions between elementary particles. Collaboration with universities will be emphasized.

Objectives

Major objectives of Argonne's work in high energy physics are as follows:

- Maximize the output and impact of new physics generated from the Laboratory's experiments.
- Complete the demonstration of the Argonne Wakefield Accelerator and exploit the facility for further experiments in advanced acceleration technology.
- Advance the technology of high energy physics detectors by improving existing detector devices and inventing new ones.
- Improve theories of particle physics and expand understanding of experimental consequences.

Issues and Strategies

High energy physics experiments are conducted in most cases by large international collaborations. Increasingly, accelerator or collider facilities are unique and are not duplicated elsewhere in the world. Accordingly, Argonne's work in high energy physics is increasingly conducted at foreign accelerators, as well as those in the United States. Data taking in the ZEUS experiment at the German DESY laboratory began in 1992, and ZEUS continues to provide unique data from high energy electron-proton collisions. In 2001, a major luminosity upgrade was completed for ZEUS and related experiments, permitting a new focus on extreme values of kinematic variables where rates are low. Currently under way is fabrication work on a detector for the Large Hadron Collider (LHC), which is being constructed at the CERN Laboratory in Switzerland. Argonne researchers have established leadership roles in the ATLAS (A Toroidal LHC ApparatuS) detector, one of two major detectors planned for the LHC (and unrelated to the ATLAS facility located at Argonne). The U.S. government has a formal agreement with CERN that details the scope of U.S. participation in the LHC and the level of funding to be provided by DOE and the National Science Foundation. Some work on the ATLAS detector will shift to preinstallation and installation activities toward the end of FY 2002. The detector is expected to begin taking data in 2006.

Argonne will be carefully considering expansions or new directions for many of its programs in high energy physics, in order to preserve their effectiveness in the next decade. Argonne researchers are playing leading roles in the MINOS (Main Injector Neutrino Oscillation Study) experiment, a long-baseline study of neutrino oscillation, employing a neutrino beam from the new Fermilab main injector. MINOS is now in the construction phase. The "far" detector is to be underground, adjacent to the current Soudan 2 detector in Minnesota. Argonne has primary responsibility for scintillator module construction at multiple sites and specific responsibility for developing and fabricating near-detector scintillator modules and front-end electronics. The Laboratory is also coordinating installation of the far detector at the Soudan Mine. First data from the detector are expected in FY 2004. A major upgrade of the CDF (Collider Detector at Fermilab) began taking data with the upgraded Fermilab Tevatron in 2001. Argonne's Wakefield Accelerator R&D program is now preparing for the second phase of its demonstration program; in order to explore ways of using this new accelerator technology in future experimental facilities, the Laboratory is discussing possible collaborations and alliances with researchers at other institutions.

The ATLAS detector at the CERN Laboratory in Europe is designed to solve the fundamental puzzle concerning the mechanism of electroweak symmetry breaking and the origin of mass. Calorimeter fabrication began in FY 1999 and must be completed by late FY 2002, when installation begins at CERN. Argonne is currently contributing to the design and prototyping of the trigger for ATLAS. System components will be built, tested, and commissioned during the coming five years. Development of the computing system for the ATLAS detector began as a new task in FY 2000 and became fully integrated with other U.S. work on ATLAS during that year. In collaboration with other U.S. and foreign ATLAS institutions, Argonne is taking the lead role in developing core data management software, as well as calorimeter-specific software.

In theoretical high-energy physics, funding limitations have prevented the addition of junior researchers at appropriate intervals. With DOE, Argonne will explore means of adding one or more early career theorists, particularly in the area of neutrino physics.

Discussed below as programmatic initiatives are future efforts on the ATLAS detector software task and R&D toward a linear electron-positron collider and associated detector.

Initiative: ATLAS Detector Software Development

Provision of computing systems to support U.S. participation in the ATLAS detector at CERN's LHC was not addressed in the original combined LHC project agreement. This task includes the provision of computing, storage, and networking facilities in the United States to support simulation and analysis of ATLAS data by U.S. researchers, as well as software development by U.S. collaborators that will contribute to the overall ATLAS software system. Argonne, in cooperation with the University of Chicago, is leading the development of a major part of the software for which the United States has responsibility. The detailed work plan designates Argonne as the lead U.S. institution for development of a central database or database management software.

Resources required for work on ATLAS software are summarized in Table IV.2. Funding is sought from the High Energy Physics Program (KA-04).

Table IV.2 ATLAS Detector Software Development ($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	1.5	2.0	2.0	2.0	2.0	2.0	1.5
Capital Equipment	0.2	0.4	0.6	0.6	0.2	0.2	0.1
Construction	-	-	-	-	-	-	-
Total	1.7	2.4	2.6	2.6	2.2	2.2	1.6
Direct Personnel	7.0	10.0	10.0	10.0	10.0	10.0	7.0

Initiative: Linear Collider Accelerator and Detector Technology

In January 2002, a subpanel of the DOE-National Science Foundation High Energy Physics Advisory Panel gave highest priority to construction of a linear electron-positron collider in the energy range 500-1,000 GeV. This collider will complement the LHC by having sensitivity to a similar energy and mass range for new phenomena but qualitatively different measurement and identification abilities.

Success in building and exploiting this new collider depends on solving a number of design issues and choosing between two major accelerator technology alternatives, based on either warm or superconducting radio frequency cavities. Substantial R&D is also needed on the detector for the new collider, in order to optimize its ability to reconstruct events with the required precision. Argonne plans R&D on both the accelerator and the detector. For the accelerator, the Laboratory will use its world-class expertise in photocathode guns and electron beam optics. For the detector, the Laboratory proposes a new hadronic calorimeter technology based on resistive-plate chambers, which will be used with the energy flow approach to calorimetry being explored with the ZEUS detector.

Resources required for Argonne's work on this initiative are summarized in Table IV.3. Funding is sought from the DOE High Energy Physics Program (KA-04).

Table IV.3 Linear Collider Accelerator and Detector Technology ($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	0.2	0.5	0.8	1.0	1.0	1.0	1.0
Capital Equipment	-	0.2	0.3	0.3	0.3	0.3	0.3
Construction	-	-	-	-	-	-	-
Total	0.2	0.7	1.1	1.3	1.3	1.3	1.3
Direct Personnel	1.0	2.0	4.0	5.0	5.0	5.0	5.0

f. Mathematics, Computing, and Information Sciences

Situation

Many new scientific applications areas become tractable when computers operate at petaflops per second. These areas include computational biology and environmental science, multidisciplinary design, first-principles simulations in chemistry and materials science, and integrated modeling of Earth systems. Accordingly, the U.S. government has established the long-term goal of improving the large-scale computing systems needed for research and defense into the petaflops performance regime.

Developing and efficiently using petaflops computers by 2006 will require substantial advances in hardware, algorithms, systems software, and related enabling technologies. The hardware challenge alone is formidable. Although commodity clusters of computers have proved useful for large-scale scientific systems, such clusters appear to be incapable of scaling effectively to the petaflops regime. Instead, various point designs must be explored, such as cluster-on-a-chip technology and strategies involving integrated processors in memory or systems on a chip. Close collaboration with computer vendors will be critical to overcoming the hardware challenge.

Petaflops computing will also require a strong software infrastructure. Simple enhancements to existing software will not suffice. Researchers will need to explore new strategies, such as the co-development approach, which links development of systems software and compilers. Moreover, novel interfaces must be developed to integrate petaflops computing into the emerging national computational grids, and high-level tools will be needed so that users can quickly and seamlessly move applications from the workstation to a large-scale facility. A further major challenge will be the development of systems integration strategies that enable system scalability, from teraflops to petaflops, while still using the same hardware and software elements.

Vision and Goals

Computing science contributions at Argonne over the next five years will center on scalable computational resources, expertise in strategic applications areas, solutions to major scientific and engineering problems, remote sharing of instrumentation and immersive visualization facilities, and collaborative teams of computational and computer scientists.

Key to realizing this vision are world-class supercomputing and networking resources, complemented by world-class algorithms, tools, and software. The Laboratory will explore diverse avenues to achieving high performance, including scalable-cluster technology, distributed supercomputers, and teraops computer systems. The goal is to offer terascale computing, with an order-of-magnitude increase in bandwidth and a comparable decrease in latency.

Argonne researchers also will make seminal contributions to the software base for the next generation of problem-solving environments by addressing a wide range of challenges related to collaborative and distributed computing. Emphasis will be on open-source tools that make it easy for scientists to obtain codes, methods, and libraries and to work together in tackling large-scale scientific problems. In addition, Argonne will participate in large-scale joint ventures — such as the National Computational Science Alliance in the Partnerships for Advanced Computational Infrastructure — in order to research, develop, and validate the technologies needed to support applications scientists.

Objectives

Argonne has established the following specific objectives for its mathematics, computing, and information sciences program:

- Encourage Laboratory-wide strategic computational science applications that advance the frontiers of science in such areas as computational chemistry, computational fluid dynamics, and bioinformatics.
- Contribute importantly to the nation’s enabling computing technologies by developing the software tools, distributed

computing, visualization, and numerical libraries needed to solve the most challenging scientific problems.

- Develop computational methods that enable better predictions in critical policy areas, such as climate modeling.
- Integrate efforts in advanced computation (including computer science, mathematics, and computational science) with experimental and theoretical research.
- Explore new technologies by anticipating needs and advancing the state of the art of large-scale computing in ways that make researchers more productive.

Issues and Strategies

Argonne researchers in mathematics and computer science continue to be at the forefront of scientific computing, leading efforts to develop new paradigms and technologies. One important area of work is distributed computing systems, where coupling of workstations and parallel computers, large databases, virtual-reality devices, and other resources worldwide promises tremendous advances in scientific problem solving. The Laboratory's aggressive pursuit of ways to enable distributed collaborative science applications includes (1) the Distributed Systems Laboratory, which is exploring computational grids for science and engineering, and (2) the Futures Laboratory, which is developing the Access Grid for collaborative tutorials and conferences.

The recent federal program Scientific Discovery through Advanced Computing offers increased funding for the computing sciences. Argonne researchers plan to make major contributions to this program by establishing national collaboratories and high-performance networks, developing centers for integrated software infrastructure, and performing fundamental research in computational science. Essential to the success of such efforts is access to world-class production and experimental computing facilities, as proposed in the major Laboratory initiative Petaflops Computing and Computational Science (Section III.A.4).

Argonne also proposes a major reorganization and expansion of its applied mathematics program in response to objectives established by DOE's Office of Advanced Computing. Areas of investigation will include optimal control, multiscale modeling, and development of petaflops-class algorithms and technologies. In addition, major new thrusts will be initiated in such areas as data grids and collaboratories, modeling and analysis tools for molecular and cell biology, systems software and architecture research for petascale systems, and networking research test beds.

Progress in computer and communications technologies has set the stage for major advances in scientific problem solving. Argonne has a tremendous opportunity to contribute to these advances, but the opportunity will be lost without major investments in computational modeling and simulation. Critical to the Laboratory's efforts will be partnerships involving teams of computer scientists, computational scientists, and hardware developers from national laboratories, universities, and the commercial sector. This path is clearly the most effective one to an effective petaflops system that is balanced and addresses the needs of the many applications areas that can benefit.

g. Intense Pulsed Neutron Source

Situation

The IPNS has operated as a national user facility since its commissioning in 1981. Among DOE neutron sources, it has one of the largest user programs: in both FY 2000 and 2001, between 230 and 240 scientists conducted a total of approximately 400 experiments. Moreover, the IPNS is DOE's most cost-effective neutron source. Its high scientific productivity and cost-effectiveness have been noted frequently by national and international committees. In February 2001 that evaluation was reinforced by DOE's Basic Energy Sciences Advisory Committee (BESAC), which strongly recommended increasing annual IPNS funding by $9 million in order to (1) improve the accelerator, targets, moderators, and available instruments and (2) expand the facility's research program. The IPNS currently provides 13 neutron scattering instruments, as well as facilities for studying radiation effects. IPNS operated for 25 weeks in

FY 2001, and it is scheduled to operate for 27 weeks in FY 2002.

Vision

The IPNS will function as a reliable and accessible user facility for neutron scattering research and as a successful developer of targets, moderators, and state-of-the-art neutron scattering instrumentation. Staff will help qualified users conduct world-class condensed matter research that addresses a wide range of questions important to both science and technology. Through enhancements, the IPNS will maintain leading-edge capabilities in neutron scattering. Through expanded collaboration with other Argonne facilities, such as the APS and the CNM (Section III.A.1), the IPNS will further increase its scientific productivity.

Issues and Strategies

The IPNS has historically been severely oversubscribed, understaffed, and underfunded. The additional $4 million in IPNS operating funds included in DOE's Scientific Facilities Initiative beginning in FY 1996 now allows approximately 25 weeks of operation per year, with a full complement of instruments serving users. A 16% increase in FY 2002 operating funds from DOE, along with an anticipated 7.5% increase in FY 2003, will enable the IPNS to begin work toward enhancing its instruments. Improved instruments are expected to attract about 70% more users each year, or 400 rather than 240.

Neutron scattering in the United States will be in a state of flux for the next decade. Currently, two DOE facilities and a facility of the National Institute of Standards and Technology (NIST) provide neutrons: the IPNS, the Los Alamos Neutron Science Center (LANSCE) at Los Alamos National Laboratory, and the NIST Center for Neutron Research in Gaithersburg, Maryland. A major upgrade of the High Flux Isotope Reactor (HFIR) facility at Oak Ridge National Laboratory is currently under way, and construction of the 1-MW world-class Spallation Neutron Source (SNS), also at Oak Ridge, is scheduled for completion in FY 2006, with full user access scheduled for FY 2008. Consequently, over the next six years the IPNS will evolve from a major national source of neutrons for U.S. users to a medium-sized regional facility. In this environment, the role of the IPNS will be increasingly coupled to the APS and the CNM.

The role of the IPNS over the next decade in serving neutron scattering researchers and the broader scientific community is best described in terms of short-, medium-, and long-term strategies.

Short-Term Strategies (Next Three Years). The IPNS role in the early transition period is to promote growth in the U.S. neutron user community and to support the SNS project so that world-class instruments and a responsive user program are in place when that new facility is commissioned. The IPNS also must begin positioning itself for highly productive research after the SNS starts operations. These goals can be achieved through the following actions:

- Institute incremental accelerator and source upgrades, and increase the number of IPNS users during a year from 240 to 400.
- Improve IPNS instruments so as to build the facility's user base and more effectively train neutron users.
- Host the SNS instrument development team. Test SNS instrument concepts, components, data acquisition systems, and detectors.
- Contribute to the SNS project where appropriate, in the areas of target, moderator, accelerator systems, and user programs.
- Conceptualize SNS instrumentation capable of serving frontier scientific experiments in the coming decades.
- Leverage the full range of capabilities available at the CNM, the APS, and the IPNS in order to better serve facility users.
- Create joint staff appointments between the IPNS and the APS, the CNM, and the University of Chicago.

Medium-Term Strategies (Three to Seven Years). Just before SNS operations begin, the IPNS role will be to begin development of the next generation of SNS instrumentation and to operate the IPNS with upgraded instrumentation that better supports the neutron scattering community. Closer ties with the APS and the CNM will facilitate more effective utilization of neutrons and photons to investigate fundamental issues in science and technology. These goals can be achieved through the following actions:

- Continue to operate the IPNS in a very effective manner (at 95% reliability).
- Give priority to development of IPNS instruments that will be capable of world-class science after SNS startup.
- Within the IPNS, strengthen expertise for nanoscience characterization.
- Begin the design and construction of up to four SNS instruments.
- Further strengthen scientific ties to complementary U.S. facilities, starting with the APS and the CNM at Argonne. Establish further joint staff appointments with those Laboratory facilities.
- Continue leading U.S. improvements to accelerator and target/moderator operations for neutron sources.
- Develop software and methods that support remote data access and control of experiments using the Internet.

Long-Term Strategies (beyond Seven Years). After FY 2008 the U.S. neutron scattering landscape will be significantly different from today's. The brilliance of the SNS and its world-class instrumentation will make that new facility especially well suited for parametric studies and studies of very small samples. The IPNS will become a regional facility supporting both fundamental research and the development of instruments, optical devices, and detectors for neutron sources. The IPNS will be especially useful for speculative or exploratory experiments and for investigations in scientific fields where combining photon probes and neutron probes is important, such as nanotechnology, soft-matter studies, and research on magnetic materials. In addition, Argonne will work toward full instrumentation of the SNS high-powered target station and will play a lead role in building the Long Wavelength Target Station at the SNS. These goals can be achieved through the following actions:

- Commission and operate selected neutron scattering instruments at the SNS by utilizing the instrument development team concept developed by the SNS.
- Continue collaboration with Argonne research partners and with university scientists to give users the tools best suited to their fundamental research, whether located at the IPNS, the SNS, or the APS.
- Leverage complementary assets within Argonne and across the DOE laboratory system — including the IPNS, the CNM, the APS, the SNS, and the HFIR — to best serve the missions of DOE and other research sponsors.
- Provide leadership for U.S. efforts aimed at developing improved neutron optics and detectors.
- Lead the design and construction of the Long Wavelength Target Station at the SNS.

Initiative: IPNS Enhancement

Under the IPNS Enhancement initiative, Argonne proposes to improve existing instruments significantly (increasing data rates by factors ranging from 2 to 32) and to increase the number of weeks of operation to enable an expanded user community to gain experience at a pulsed source in preparation for using the SNS. These additional operations and scientific capabilities were detailed in a plan presented to the November 2000 meeting of the BESAC subpanel reviewing operations at LANSCE and IPNS. In February 2001 the Argonne plan became the first of the subpanel recommendations approved by BESAC.

Work on equipment under the IPNS enhancement plan falls primarily into (1) accelerator upgrades and spare parts, (2) improvement to the moderator and reflector, and (3) instrument enhancements:

1. Reliability will be maintained above 95% by upgrading aging accelerator systems and obtaining spare parts in FY 2002. In addition, a 30% increase in neutron production will be achieved through utilization of secondary

harmonic technology in the accelerator system.

2. Judicious choice of replacement materials can improve neutron yield by a further 20%. This work is currently scheduled for 2003.

3. The performance of all IPNS instruments can be increased significantly through various enhancements, such as more detectors, better data acquisition systems, neutron guides, and new ancillary equipment. Implementation of these enhancements over the next four years will improve data rates by factors as great as 32, allowing many IPNS instruments to be competitive with those at the world's best pulsed neutron source, ISIS in the United Kingdom.

Resources required for the IPNS enhancement initiative are summarized in Table IV.4. Funding will be sought from DOE-BES (KC-02).

Table IV.4 IPNS Enhancement
($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	1.6	2.6	3.6	4.6	5.3	6.0	6.8
Capital Equipment	0.6	1.8	2.3	2.0	1.0	-	-
Construction	-	-	-	-	-	-	-
Total	2.2	4.4	5.9	6.6	6.3	6.0	6.8
Direct Personnel	6.0	8.5	11.0	13.5	13.5	13.5	13.5

h. Biosciences

Situation

The sequencing of the human genome is approaching completion, and over 200 other genome sequences are either completed or in process. With these accomplishments, biology has reached a turning point at which complete enumeration of the genes used by an organism is within reach. The challenge now is to interpret this information to construct a detailed, coherent, complete view of living organisms and to use this view to develop powerful methods for manipulating and engineering biomolecular systems and predicting their responses to environmental stimuli. The key to such detailed control of biomolecular systems lies in a complete mapping of the activities of the gene products of a cell that cooperate to perform all cellular processes. The information required to characterize these processes is embedded in the spatiotemporal distribution of gene products and metabolites across multiple length scales.

In coming years, progress in the biological sciences will depend increasingly on interdisciplinary interactions with computational, physical, chemical, and materials scientists. Implementation of high-throughput techniques for biochemical and biophysical characterization of biomolecular systems will make it possible to address experimental challenges that are now unbroachable. Huge volumes of data will be required. Cataloging and preserving those data and then extracting maximum information will present a significant challenge in database design and maintenance. In the longer run, integrating the data into a complete view of cellular (and, ultimately, organismal) behavior will require novel approaches to simulating complex systems. Computation will come to dominate the biological sciences in the 21st century. This approach to genome-scale analysis of biological function, now widely referred to as systems biology, involves the fusion of functional genomics with high-end computational simulations of the molecular behavior within biomolecular systems.

Vision and Goals

Argonne will move toward a leadership position in postgenomic biology by creating a model program for the comprehensive functional analysis of genomes. The Functional Genomics initiative (see Section III.A.3) will take advantage of the Laboratory's strong programs in the physical, chemical, materials, and computational sciences to build, along with biosciences, a uniquely interdisciplinary program for post-genomic biology. Partnership with computational scientists will develop a systems biology capability that will be well positioned for the comprehensive analysis of the behavior of microorganisms that are relevant to DOE's science mission.

Experimental facilities at the APS and world-class computational resources will be integral parts of Argonne's program for genome-wide structural and functional characterization of organisms — a program that will be centered around the Laboratory's quickly growing effort in structural and functional genomics. Revolutionary approaches to currently intractable problems will be explored in collaboration with Argonne physicists, chemists, and engineers. Programs in bioinformatics, nanobiotechnology, and combinatorial biology will engage scientists at both the Laboratory and the University of Chicago. The goal is a focused program aimed at developing and using high-throughput experimental and cutting-edge computational capabilities for the complete functional characterization of whole genomes.

Objectives

Argonne's Functional Genomics initiative will grow around the Laboratory's current structural and functional genomics programs by taking advantage of both resources supporting the current program and other resources at the APS and across the Laboratory. The initiative will greatly strengthen cross-disciplinary interactions aimed at creating revolutionary approaches to currently intractable problems.

Argonne's major objectives in biosciences are focused on its major Laboratory initiative, Functional Genomics (Section III.A.3), elements of which include the following ongoing and novel efforts:

- *Structural Genomics.* Develop a scientific program aimed at deepening understanding of the relationship between protein structure and function — a program centered on current efforts to characterize to atomic resolution the three-dimensional structure of all gene products and to use that structural information to develop better understanding of the function of each gene product.

- *High-Throughput Protein Production and Crystallization.* Argonne's current use of robotics for high-throughput expression of proteins will provide milligram quantities of hundreds of proteins for functional analysis. In parallel with crystallization efforts, these proteins will be analyzed by using functional proteomics, combinatorics, and small-angle x-ray diffraction. The robotics expertise of Laboratory scientists will be exploited to develop techniques for high-throughput biochemical and biophysical analyses. Upgraded robotics capabilities for the rapid and efficient production of diffraction-grade crystals of biological macromolecules will eliminate the most severe bottleneck in the Laboratory's structural genomics work.

- *Revolutionary Approaches to Membrane Protein Crystallization.* The 30% of proteins that are integral components of cellular membranes cannot be investigated by using the techniques that are successful in crystallizing other proteins. In collaboration with physical and chemical scientists, Argonne will explore revolutionary approaches to the crystallization and biochemical analysis of these proteins.

- *Program for Combinatorial Biology.* Mapping of protein-protein and protein-ligand interactions is one of the most powerful methods for the functional analysis of macromolecules. A comprehensive program in combinatorial biology is being developed to take advantage of the huge potential of this approach for the functional analysis of whole genomes. Furthermore, a program for the high-throughput production of affinity tags will be developed to aid in the purification and functional analysis of gene products. This program will use combinatorial libraries of proteins and peptides displayed on the surfaces of viruses and bacteria and will screen these libraries for desired functionalities.

- *Program in Nanobiotechnology.* Argonne materials scientists and biologists will cooperate to develop a new program in nanobiotechnology that will explore the creation of bio-inspired nanostructures and bio-compatible materials, as well as the structural analysis of complex biological materials.

Issues and Strategies

Argonne is uniquely positioned to take advantage of the extraordinary opportunities developing in postgenomic biology. Through multidisciplinary collaborations among scientists across the Laboratory and at the University of Chicago, Argonne will seek leadership in newly defined areas of the biological sciences and will explore revolutionary approaches to a number of currently intractable problems in structural and cellular biology.

The core of Argonne's bioscience efforts is work in structural genomics to establish high-throughput macromolecular crystallography and its use for enumerating all existing protein structural motifs. This work has motivated initiatives in high-throughput crystallization of macromolecules and high-throughput expression of proteins in bacterial hosts. Building on the Laboratory's existing robotics expertise, these initiatives will provide a further base for developing robotics for rapid biochemical and biophysical assays of protein structure and function. Argonne's existing structural genomics efforts are tightly focused on crystallographic studies, and augmentation in the indicated directions is a priority.

In general, development of new interdisciplinary interactions across the Laboratory and with the University of Chicago will drive Argonne's planned initiatives in the biosciences, where DOE and the National Institutes of Health (NIH) will be major funding sources. The Functional Genomics initiative (Section III.A.3) directly addresses the goals of DOE's new Genomes to Life program. In addition, important funding from the state of Illinois is being sought to enhance the planned program in high-throughput protein production and crystallization. A key complementary strategy is development of cooperative agreements with biotechnology companies for joint development of novel methodologies.

Argonne initiatives in the biosciences will build from four parallel and complementary efforts in macromolecular crystallography that are currently being pursued: (1) The capabilities of the existing DOE-funded Structural Biology Center are being enhanced significantly through support from NIH. The Midwest Center for Structural Genomics will receive from NIH approximately $5 million per year for development of high-throughput macromolecular crystallography. (2) In partnership with this effort, Argonne is also working with NIH to develop a second APS sector for macromolecular crystallography. (See Section S1.C for discussion of these NIH-supported efforts.) (3) To facilitate this work, a laboratory complex for biostructure research has been constructed at the APS with joint DOE and NIH funding (see Section IV.A.1.a). (4) Argonne is also working with the state of Illinois on plans to construct an Accelerated Protein Production and Crystallization Facility at the APS, which is to include development of an additional APS sector for structural genomics and macromolecular crystallography. Close partnerships among these four efforts will enable significant economies of scale, facilitating rapid improvement in the understanding of structure and function in proteins.

Around these significant efforts in structural and functional genomics and crystallography, Argonne is building its Functional Genomics initiative. Research on genome-wide analysis of the structure, assembly, and operation of gene products is greatly expedited by the use of large-scale, high-throughput capabilities for analyzing intermolecular interactions and other biochemical and biophysical parameters of macromolecular complexes. This initiative will establish the resources needed for comprehensive studies of biomolecular machines, interface this effort with the Laboratory's ongoing work in structural genomics, and use the resulting capabilities to characterize the molecular machines critical to cellular processes in all organisms.

i. Environmental Research

Situation

Environmental issues continue to be a leading national concern, reflecting population growth, economic development, and the environmental legacy of past activities and practices. The focus is shifting from effluent control technologies and associated regulation toward waste and resource management, site remediation and long-term stewardship, facility decontamination, and global environmental issues. Basic and applied research leading to more cost-effective environmental technologies and practices is increasingly important. Moreover, new technology and information — such as geographic information systems, computer imaging, and satellite survey data — have created opportunities to address hitherto intractable environmental problems.

Vision

Argonne will provide national and international leadership in key areas of environmental research by developing innovative and cost-effective solutions to high-priority environmental problems, such as carbon cycling and carbon sequestration, climate change and air quality, biogeochemical cycling, and improved site characterization and remediation. Laboratory researchers of recognized professional standing, complemented by state-of-the-art facilities and instruments, will address problems at the frontiers of environmental science that are technically challenging, broadly relevant, and unlikely to be resolved in a timely fashion through private-sector R&D alone.

Objectives

Central objectives of environmental research at Argonne are as follows:

- Make significant, growing contributions to three environmental grand challenges: (1) biogeochemical cycling, (2) atmospheric particulates and aerosols, and (3) a hydrogen-based energy system.
- Develop synchrotron-based techniques for molecular environmental science, based on the high-brilliance x-rays of the APS.
- Develop fundamental studies of soil carbon characterization and transformation in order to understand and quantify carbon sequestration as a method for controlling atmospheric carbon dioxide levels.
- Further expand the Atmospheric Boundary Layer Experiments (ABLE) site as a facility generating data required for research on climate change, including the exchange of carbon and water between the atmosphere and terrestrial ecosystems.

Issues and Strategies

Argonne has significant core capabilities in bioprocessing; ecology; modeling and measuring environmental pathways; atmospheric physics and chemistry; developing "clean" technologies; control and remediation technologies; and development of decision models for rapid, cost-effective remediation of DOE sites. This foundation provides important opportunities for fruitful integration of applied environmental studies with fundamental capabilities in physics, chemistry, biology, and mathematics. Building on this foundation, the Laboratory plans to establish broad, multidisciplinary research teams for large-scale studies in environmental science.

Cost-effective resolution of the important environmental issues facing DOE, the nation, and the world requires the integrated application of multiple scientific disciplines. Argonne believes that the future of environmental research at the national laboratories lies in increased emphasis on basic and applied research conducted by multidisciplinary teams able to exploit fully major research facilities and other unique capabilities. Better solutions to environmental problems can be achieved both by expanding the knowledge base and by applying what is already known more effectively. The initiative Grand Challenges in Environmental Science at the end of this area plan expands on this theme.

In the area of atmospheric science, Argonne is building on its existing capabilities in atmospheric science, remote sensing, advanced computation, information processing, and important observational efforts in climate change, atmospheric chemistry, carbon cycling, and hydrology. Facilities are managed with the overall objective of making available to all qualified users continuous, long-term observations from state-of-the-art instruments distributed over a large area in a meteorologically important region of the country and thereby to create a key national asset for progress in atmospheric and hydrospheric research. Data from Argonne's ABLE site contribute to DOE's AmeriFlux (carbon flux) and Environmental Meteorology research programs and to the National Aeronautics and Space Administration's land surface hydrology program. The ABLE site is now also the study site for a pilot program demonstrating DOE's capabilities in a new national Water Cycle Initiative.

At the end of FY 2000, Argonne assumed responsibility for operations and oversight for all three Cloud and Radiation Testbed facilities of the DOE-BER Atmospheric Radiation Measurement Program. The Laboratory's operating resources for Environmental Processes (see KP-12 in Chapter VI) now include substantial DOE funding for redistribution to other national laboratories, universities, and subcontractors.

Argonne conducts research for the Atmospheric Chemistry and Environmental Meteorology components of the DOE-BER Atmospheric Sciences Program and provides the lead scientist for Atmospheric Chemistry. The Laboratory participates in collaborative field campaigns that gather information on the sources and fates of oxidants and particulate matter in the lower atmosphere and on associated meteorological processes. Associated DOE research addresses numerous scientific challenges regarding the effects of energy-related trace chemicals on local and regional air quality and on climate. The work at Argonne emphasizes dry air-surface exchange, which affects the budgets of chemicals in the lower atmosphere; chemical transformations leading to oxidant and particle formation; and physical processes that transport materials vertically and horizontally in the lower one or two kilometers of the atmosphere.

The central goal of Argonne's work in synchrotron-based environmental science is an atomic- and molecular-level understanding of structure and processes in environmental systems. One set of studies considers mineral-fluid interactions and the mechanisms by which contaminant elements become bound to mineral surfaces. Other studies focus on developing synchrotron-based imaging techniques for environmental and biological samples and on understanding the speciation, binding, distribution, and mobility of heavy metals and radionuclides in soil-fluid-biota systems. These multidisciplinary efforts build on the Laboratory's widely recognized research at the forefront of molecular radiation science and environmental science and involve several new internal and external collaborations. See the focused initiative Synchrotron Environmental Science at the end of this area plan.

Argonne is building and strengthening ongoing programs in site characterization and soil ecology. The Laboratory continues its R&D on environmental tools such as QuickSite®, a methodology that has become the basis for the American Society for Testing and Materials standard for expedited site characterization.

In the area of soil ecology, studies are under way on the importance of soils in sequestration of carbon dioxide and, in conjunction with the synchrotron-based environmental research, on the molecular-level processes that result in soil aggregation.

Argonne is participating in two new research centers at the University of Chicago that have grown from long-standing collaborations. The Joint Argonne-University of Chicago Center for Environmental Science will investigate the effects of urbanization and regional climate variability on human health, while the Center for Integrating Statistical and Environmental Sciences will develop innovative statistical methods and approaches for analyzing and validating environmental data.

Initiative: Grand Challenges in Environmental Science

Numerous diverse research activities conducted throughout the Laboratory have significant environmental benefits or applications. By integrating the underlying expertise via collaboration among multidisciplinary teams, Argonne aspires to increase its impact on three nationally recognized environmental "grand challenges" that match the Laboratory's capabilities — both expertise and facilities — particularly well: (1) biogeochemical cycling, (2) atmospheric particulates and aerosols, and (3) the transition from a hydrocarbon-based economy to one based on hydrogen.

In biogeochemistry, central goals are (1) to quantify the rates of transfer of compounds to and from storage reservoirs (implying accumulation and depletion) and (2) to determine the mechanisms controlling these transfers. The most important challenge is to understand how Earth's major biogeochemical cycles are perturbed by human activities; to predict the impact of these perturbations on local, regional, and global scales; and to determine how these cycles could be restored to more natural states. Argonne teams will focus on primary and secondary interactions between the multiple elements of these problems and on the associated positive and negative feedbacks. Studies will range from the atomic level to bench scale to field scale.

Atmospheric particulates, both natural and anthropogenic, are inextricably linked to energy production and use. Such particles have significant detrimental effects on human health, play a major role in acid rain formation, and have direct and indirect radiative forcing effects that are comparable in magnitude to the effects of greenhouse gases but of opposite sign. The characteristics, distribution, and transport of such particles over long distances affect issues ranging from national security (e.g., transport of harmful spores) to general air quality (e.g., atmospheric chemical interactions). Argonne research will determine how atmospheric particles are formed, their roles in global and regional climate systems, and their relevance to chronic and acute respiratory diseases. Approaches based on materials science, chemistry, and physics are particularly appropriate for these studies.

Argonne is well positioned to investigate the potential effects of a shift from a hydrocarbon fuel infrastructure to one based on hydrogen fuel. The Laboratory can help to understand, predict, and mitigate the environmental consequences of this shift. The Laboratory's capability to study hydrogen production is particularly outstanding. Questions to be addressed will include effects of atmospheric emissions on tropospheric and stratospheric hydroxyl radical concentrations, changes in stratospheric ozone, and resulting effects on urban areas. These studies can take advantage of Argonne's strong engineering capabilities in the nuclear generation of hydrogen and in novel approaches to environmental control technologies.

This effort fits within the scope of the U.S. Global Change Research Program's FY 2003 initiative in climate change, a likely near-term source of funding. Other programs that would benefit from Argonne's pioneering approach to multidisciplinary integrated research are DOE's Genomes to Life program and DOE environmental remediation studies, such as those of the Natural and Accelerated Bioremediation Research Program and the Environmental Management Science Program. This initiative will draw on the new Joint Argonne-University of Chicago Center for Environmental Science, a formal collaboration that will perform research on environmental issues. Other potential federal sponsors are the Environmental Protection Agency, the National Oceanic and Atmospheric Administration, the National Aeronautics and Space Administration, the National Science Foundation (in collaboration with university partners), and the Department of Defense. Required resources are summarized in Table IV.5.

Table IV.5 Grand Challenges in Environmental Science ($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	-	2.0	3.6	5.6	8.0	10.0	10.0
Capital Equipment	-	-	1.0	2.0	2.0	2.0	2.0
Construction	-	-	-	-	-	-	-
Total	-	2.0	4.6	7.6	10.0	12.0	12.0
Direct Personnel	-	5.0	9.0	14.0	20.0	25.0	25.0

Initiative: Synchrotron Environmental Science

Environmental research is undergoing a technical revolution. Environmental scientists, who have long used the classical macroscale research methods of biology, chemistry, geology, and physics, are just beginning to apply the newer microscale research technologies in truly interdisciplinary studies. In the offing are immense benefits from applying recent advances in x-ray spectroscopy, scattering, and imaging. Benefits range widely, including determinations of chemical speciation and mineral-fluid interface structure in the environment, optimization of chemical sequestration technologies, characterization of soil organic matter, insight into carbon sequestration mechanisms, and improved understanding of biotic processes in extreme environmental conditions.

Demand for environmental research capability at the APS is growing rapidly. For example, the existing GSECARS user program receives many more environmental research proposals than it can accommodate with available beam time. The first Synchrotron Environmental Science workshop, held at Argonne in April 1999, strongly confirmed the growing shortage of beam time relative to worthy research proposals, despite the fact that the National Science Foundation and DOE-BES have already invested heavily in GSECARS and BESSRC beamlines that serve geoscience and environmental science. The second workshop, held in May 2002, demonstrated continued growth in the field of environmental molecular sciences and underscored the research community's need for additional beam time and optimized instrumentation.

Argonne research groups are already undertaking major projects at the forefront of synchrotron environmental science. These research projects utilize beam time at four APS collaborative access teams (BESSRC-CAT, MR-CAT, SRI-CAT, and GSECARS-CAT), as well as at the National Synchrotron Light Source and the Stanford Synchrotron Radiation Laboratory. Substantially more access to APS beam time will clearly be required for the expanded scientific program envisioned in this initiative. Development of new beamline capabilities will be pursued through partnerships with other organizations having complementary research interests.

To meet the need for additional synchrotron environmental science capabilities, Argonne has formed a partnership with the University of Chicago and the University of Notre Dame to establish a new collaborative access team at the APS that will be devoted to environmental research. This collaborative access team (EnviroCAT) is intended to provide dedicated, state-of-the-art facilities that are optimized for research on a broad range of environmental science problems. EnviroCAT will focus on developing a multifaceted microbeam facility and a microtomography facility using, respectively, insertion device and bending magnet beamlines. The letter of intent submitted to the APS program review board has been approved, and work will begin in FY 2003 to develop initial design criteria. Discussions with potential institutional partners are expected to result in additional formalized research partnerships in FY 2003.

Resources envisioned for development of EnviroCAT are described in Table IV.6. Support will be sought from DOE-BER (KP), DOE-Environmental Management (EW, EX), other federal agencies, and private sources.

Table IV.6 Synchrotron Environmental Science
($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	0.5	1.0	2.0	2.0	2.0	2.5	2.5
Capital Equipment	-	-	2.5	1.5	0.5	-	-
Construction	-	-	8.5	4.0	4.0	-	-
Total	0.5	1.0	13.0	7.5	6.5	2.5	2.5
Direct Personnel	2.0	2.0	10.0	10.0	10.0	10.0	10.0

j. Science and Engineering Education and University Programs

Situation

Argonne has maintained very active and wide-ranging interactions with the academic community throughout its existence. The activities range from programs that support science education at the high school level to mutually beneficial research partnerships between university faculty and Argonne research staff in virtually all of the Laboratory's scientific and technical areas. These activities are supported by the Laboratory, through work for non-DOE sponsors, and by DOE.

Argonne's science and engineering education programs serve faculty and students at both the university and precollege levels. Core programs at the university level provide opportunities for research participation by outstanding under-graduates and faculty, as well as opportunities for thesis research by graduate students. Argonne has become more active in unique graduate programs involving several strategic areas of interest to DOE. These programs include long-term internships and short-term training in a wide range of the Laboratory's research areas. The quality and value of these programs attract applicants from throughout the country.

As part of its education program, Argonne serves the Department of State as the host institution for U.S. participation in training programs of the International Atomic Energy Agency (IAEA). The Laboratory develops and conducts courses in peaceful applications of nuclear technology and also provides technical support to the Department of State and the IAEA.

Vision

Argonne will enrich science education in the United States through activities that involve local communities, as well as students and faculty at all levels from throughout the nation. The Laboratory will work closely with DOE and other federal agencies to promote peaceful applications of nuclear technology through collaboration with the IAEA and other international organizations.

Objectives

Argonne's primary near-term objectives in support of science education and training are as follows:

- Continue to attract a large, diverse pool of highly qualified undergraduate students to research participation programs.
- Establish the Laboratory's educational user facility as a valuable and widely used resource providing hands-on laboratory experience for science teachers in the region; enhance classroom activities through use of the Internet.
- Foster student interest in science education and science careers through a variety of outreach efforts, such as the Argonne Information Center.
- Fruitfully integrate graduate students, post-doctoral fellows, and faculty into Laboratory research programs through internships and training activities.
- Provide training programs and technical assistance to a variety of international organizations.

Issues and Strategies

For its university-level programs, Argonne plans special efforts to develop supplementary activities that will broaden the science horizons of undergraduates and provide training and research opportunities for graduate students. Programs for high school students and teachers will focus primarily on hands-on laboratory work using Argonne facilities and distance learning capabilities dedicated to educational activities. In addition, the Laboratory will continue to develop programs exploiting computer technology to enhance classroom science education. Important workshops and conferences, such as the annual Women in Science conference, will continue. International programs will focus on unique Argonne research and training capabilities.

Maintaining a sound funding base is the most important issue currently facing Argonne's educational programs. Support for participants through the Office of Science has included limited infrastructure support. DOE offices with educational and training needs have been asked to consider the advantages of focusing those activities at Argonne. The Laboratory's research divisions plan to continue their strong support for the core educational programs of research participation and thesis research at the under-graduate, graduate, and faculty levels. Support for the operating costs of programs for precollege teachers in nearby school districts and in the Chicago Public Schools will be sought from the districts themselves, as well as from the state of Illinois, agencies of the federal government, and the private sector. Laboratory overhead will support the minimal infrastructure required to manage and administer these programs.

2. Energy and Environmental Technologies

Argonne research programs serving the two DOE mission areas of energy and environmental quality are so intertwined that this section includes area plans related to both.

a. Advanced Nuclear Technology

Situation

The May 2001 report of the National Energy Policy Development (NEPD) Group chaired by Vice President Cheney summarized its endorsement of nuclear power as follows: "The NEPD Group recommends that the President support the expansion of nuclear energy in the United States as a major component of our national energy policy." The NEPD Group further recommended reconsideration of next-generation advanced-fuel-cycle technologies: "In the context of developing advanced nuclear fuel cycles and next generation technologies for nuclear energy, the United States should reexamine its policies to allow for research, development, and deployment of fuel conditioning methods (such as pyroprocessing) that reduce waste streams and enhance proliferation resistance."

In view of these and other recommendations of the NEPD Group, Argonne plans to accelerate its efforts to advance nuclear technology, in order to ensure that nuclear energy can fulfill its promise as a sustainable, clean, safe, long-term energy source, free of carbon dioxide emissions. To this end, Argonne proposes in Section III.B.1 the major Laboratory initiative Advanced Nuclear Fuel Cycle. At the conclusion of this area plan, the Laboratory also proposes expansion of its existing R&D on nuclear technology, which supports current nuclear technologies, as well as those of the near future and the longer-term future.

For more than a half century, Argonne has been a world leader in the development of nuclear energy. The Laboratory's staff has extensive expertise in the full range of disciplines associated with nuclear reactor technology, and a full complement of experimental facilities is in place, representing many hundreds of millions of dollars of national assets. Currently, Argonne's nuclear technology R&D focuses primarily on (1) the Nuclear Energy Research Initiative (NERI), which aims at innovative reactor concepts, nuclear science, and nuclear technology; (2) the Nuclear Energy Plant Optimization (NEPO) program, which addresses critical technology issues associated with existing nuclear power plants; (3) the Advanced Accelerator Applications (AAA) program; (4) the Generation IV program, which aims at a new generation of nuclear energy systems to be deployed by 2030; and (5) operation of the International Nuclear Safety Center, intended to improve the safety of nuclear reactors worldwide through collaborative R&D programs and in-depth safety analysis, with primary attention to Soviet-designed reactors and the countries operating those reactors.

In partnership with the Idaho National Engineering and Environmental Laboratory (INEEL), Argonne serves as lead laboratory for Nuclear Reactor Technology for the DOE Office of Nuclear Energy, Science and Technology (DOE-NE). The primary mission for the lead laboratories during FY 2001-FY 2003 is to lead formulation of a "technology development road map" for the Generation IV nuclear energy systems program, with broad domestic and international participation.

Goals

The goals of Argonne's nuclear technology program are to develop and demonstrate innovative nuclear reactor systems and associated fuel cycles that will ensure that nuclear energy can fulfill its promise as a sustainable, long-term, emission-free source of energy; to aggressively pursue solutions for the important technical issues associated with the use of nuclear energy, both domestically and internationally; to help DOE identify and implement technology development programs that will increase the contribution of nuclear energy to a sustainable global energy supply; and to maintain a set of technical capabilities in nuclear science and technology — including both expertise and infrastructure — sufficiently broad and deep to address a full range of national needs.

Strategies

Key strategies for Argonne's nuclear technology programs include the following:

- Undertake the major Laboratory initiative Advanced Nuclear Fuel Cycle, including nuclear system R&D and design studies carried out in concert with the Generation IV program and the demonstration of an advanced fuel cycle. (See Section III.B.1.)
- Continue to participate in the NERI, NEPO, and Generation IV programs; apply Argonne's nuclear expertise and unique facilities to current, near-term, and longer-term future nuclear technologies; and apply Laboratory expertise to critical issues affecting the continued safe and efficient operation of existing nuclear power plants.

- In partnership with INEEL, serve as lead laboratory for reactor technology for DOE-NE.

- Within Argonne's areas of special expertise, participate in advanced technology R&D programs such as the AAA program.

Argonne plans a number of important new directions for its work in nuclear R&D that will support the above strategies:

- *Transient Testing at TREAT*. Argonne has begun work to reactivate the Transient Reactor Test Facility (TREAT) in order to carry out various experiments requiring a reactor capable of producing controlled transients. Though TREAT can be restarted within existing budgets, potential future testing missions will require additional resources. These missions might include testing the safety of fuel containing recycled actinides, testing the safety of advanced fuel concepts that might arise from the Generation IV program, or testing current or new fuel designs for commercial light-water reactors.

- *Advanced Fuels Development*. Argonne proposes to develop advanced fuels for power reactors, research reactors, and test reactors. Programs such as NERI and Generation IV have fostered discussion of various system configurations, but a common feature is a new fuel design. Of particular interest are metal and metal matrix dispersion fuels. Guided by system studies and technology road maps, Argonne will pursue these fuel development options and others.

- *Materials Development for Nuclear Power*. Materials R&D is important for supporting the current fleet of operating nuclear power plants, as well as for developing future innovative nuclear systems. Future nuclear power plants are likely to operate at higher temperatures and have unique corrosion environments, so advanced structural materials will be necessary. Argonne will undertake both fundamental and applied work to (1) investigate improvements in the performance and production of materials potentially applicable to nuclear power, (2) establish the capability to use modern production and analytical techniques, (3) screen new materials for likely performance in a nuclear environment, and (4) perform prototypic testing of promising advanced materials. Research aimed at both near-term and longer-term applications is proposed.

- *Post-Operation Evaluation of EBR-II Materials and Components*. A complete knowledge of the condition of Experimental Breeder Reactor-II (EBR-II) materials and components will facilitate future reactor decommissioning, life extension for current reactors, and the design of advanced reactors. In order that these valuable data are not lost, Argonne proposes significantly expanded examination of EBR-II materials and components.

- *Severe-Accident Management Technology*. Severe-accident research addresses the question of what could be done at a nuclear power plant if a core melt accident were to occur. The Laboratory's facilities for conducting severe-accident experiments have been designated an international reactor safety R&D facility by the Organization for Economic Cooperation and Development (OECD). A new research program investigating interactions between concrete and a molten reactor core is now under way. Argonne seeks continued funding for this program, whose costs are shared with international partners under OECD auspices. (See Section S1.E.5.)

- *Advanced Modeling and Simulation for Nuclear Applications*. Argonne proposes expanded work in advanced modeling and simulation for nuclear technologies. The first part of this work focuses on developing and implementing numerical methods on state-of-the-art parallel computers and workstation clusters, so that today's computing technology can be applied to improving nuclear reactor analysis. The second part focuses on machine reasoning, automated pattern recognition, and system modeling based on learned input-output relationships.

b. Energy and Industrial Technologies

Situation

Argonne develops innovative, efficient, cost-effective nonnuclear energy technologies and industrial technologies. Emphasis is on advanced transportation (discussed separately in Section IV.A.2.c), "industries of the future" identified by DOE, superconductivity, and fossil fuels and carbon management. The program also coordinates the Laboratory's development of partnerships with private companies in these areas.

"*Industries of the Future.*" Process industries convert raw materials into ingredients useful for fabrication and assembly in the automotive, electronics, aerospace, construction, and similar industries. The process industries account for approximately a third of U.S. energy consumption, at an energy cost of about $100 billion each year. Six of the major process industries — chemicals, forest products, glass, ceramics, metals, and petroleum refining — account for 78% of all industrial energy use, generate 95% of manufacturing waste, cause 95% of the total air pollution attributable to manufacturing, and account for more than 30% of U.S. carbon dioxide emissions. Because they use so much energy and produce so much waste, the federal government has set goals for U.S. process industries for the year 2010 in terms of energy reduction, oil displacement, cost savings, and pollution reduction.

Superconductivity. The electric power industry today faces a wide range of major challenges, including deregulation, aging infrastructure, global warming policies, and dependence on imported oil. Power wheeling across long distances puts a premium on technologies for the transmission and distribution of electric energy that are efficient and robust, and greater interconnectedness necessitates better technologies to protect against overloads and fault currents. Renewable energy sources are increasingly attractive, but solar or wind energy is intermittent and requires energy storage. High-temperature superconductivity technologies are being pursued by DOE and increasing numbers of electric power utilities and their suppliers as a promising response to many of these challenges.

Fossil Fuels and Carbon Management. A prudent carbon management strategy for the utility, industrial, and transportation sectors could significantly decrease net emissions of carbon dioxide and other greenhouse gases. An early, economical opportunity for greater sequestration may be provided by the capture of carbon dioxide at large point sources such as power plants, followed by use for enhanced oil recovery and production of methane from coal beds. Sectors of the economy that consume large quantities of fossil fuels are already adopting more energy-efficient technologies. Strategies for the economical use of less carbon-intensive fuels in existing plants and fleets may be an important bridge to more advanced technologies. However, a full assessment of policy options will require better understanding of carbon transformations "from cradle to grave," throughout current and proposed energy cycles. Argonne initiatives support DOE strategies to improve the efficiency of fossil energy technologies and to assist the utility, industrial, and transportation sectors in reducing greenhouse gas emission rates in other ways as well.

Partnering. Responding to the administration goal of improving the productivity of U.S. industry through appropriate use of national technical resources, Argonne is developing a broad range of partnerships with industrial firms on the basis of the Laboratory's leadership in many areas of science and technology. Argonne's midwestern location in the nation's industrial heartland provides exceptional regional opportunities. Partnerships with industry play an important role in shaping many Argonne R&D programs.

Vision

Argonne will develop new technologies that increase the productivity of U.S. industry and decrease its environmental impacts, particularly through increases in energy efficiency and reductions in intensity of petroleum consumption. As an integral part of pursuing its mission in science and technology, the Laboratory will continue to develop effective relationships with industry to maximize the commercial applications and benefits to the nation from its R&D.

Goals and Objectives

To implement this vision, Argonne's goals include the following:

- Exploit and expand Argonne facilities, capabilities, and core competencies, which integrate science and technology and interest both the scientific and industrial communities.
- Establish strategic partnerships with key industrial firms, large and small, in areas where applying the Laboratory's technical strengths is most likely to lead to valuable commercial successes.
- Implement effective regional outreach, capitalizing on the Laboratory's midwestern location.

Many U.S. industries are working with the federal government to ensure that federally sponsored R&D provides maximum benefits to the nation. Argonne has established the important research objectives summarized below, which are being pursued in close partnership with industry.

Industries of the Future

- Expand Argonne research benefiting the chemical industry, particularly research in the areas of recovery and reuse of polymers, development of chemicals from alternative feedstocks, catalysis, and plasma-chemical engineering.
- Further develop advanced technologies that improve petroleum refining by developing advanced computational modeling for fluid catalytic cracking to improve overall yields.
- Working with an industrial equipment supplier and a paper industry manufacturer, develop the multiport dryer technique, already demonstrated through proof of concept, into a prototype demonstration unit.
- Maintain the momentum of current research on metals recycling; expand work on instrumentation, materials, and fabrication technologies for the steel, aluminum, glass, and metal casting industries.
- Target key technical hurdles where unique Argonne capabilities and facilities can be used to advantage; for example, use the APS and the IPNS for critical materials studies that will enable the development of inert metal anodes for aluminum smelting.
- Advance the development of nearly frictionless, nontoxic carbon coatings for moving parts (such as oilless bearings, spacecraft mechanisms, rolling and sliding gear systems, and bearings for ultrahigh-vacuum instruments like x-ray tubes), while contributing more broadly to tribology.
- Expand Argonne research benefiting the glass industry by means of multiphase computational fluid dynamics modeling of glass furnaces; develop new techniques for recycling glass with minimal effect on product quality.

Superconductivity

- Maintain core work on the development of superconductors that is sufficiently large to sustain rapid technical development and foster extensive interactions with industrial companies and universities.
- Continue Argonne's contributions to the development of the second generation of high-temperature superconductors, building on earlier successes with powder-in-tube technology.
- Work with the manufacturers of high-temperature superconducting wire (such as American Superconductor Corporation and Intermagnetics General Corporation) to help advance manufacturing processes.
- Collaborate with system manufacturers (such as Boeing, Southwire, and S&C Electric Company) to develop and demonstrate energy-efficient products for the electric power industry, such as flywheels for energy storage, fault current limiters, electric motors, and transmission cables.
- Collaborate with other national laboratories and industrial partners to develop textured buffer layers — such as MgO, YSZ, Y_2O_3, and CeO_2 — for yttrium-based superconductor films.

Fossil Fuels and Carbon Management

• Expand and help coordinate the development of technologies that are cost-effective and highly efficient, emit smaller net amounts of greenhouse gases, and reduce environmental impacts in the utility, industrial, and transportation sectors; establish emissions inventories for promising technologies and form industrial partnerships to pursue technology development.

• Advance petroleum refining technology by developing (1) catalysts for upgrading heavy crudes, residuum, and distillates and (2) catalytic processing to produce ultraclean low-sulfur transportation fuels through heteroatom removal.

• Investigate opportunities for sequestering carbon dioxide derived from advanced fossil fuel energy systems and from retrofitting technology to the large number of existing long-lived electric generation plants.

• Improve understanding of terrestrial and oceanic responses to natural and anthropogenic changes in atmospheric concentrations of greenhouse gases.

• Develop a center for research on biogeochemical cycling of elements.

• Expand R&D on noncarbonaceous hydrogen production.

• Extend Laboratory breakthroughs in ceramic membrane technologies to advance the development of economical processes for separating oxygen from air and hydrogen from mixed gases (which are critical technologies in the use of remote natural gas and in the efficient refinery production of clean transportation fuels, respectively).

Issues and Strategies

Industry. Through the auspices of the DOE Office of Industrial Technologies, Argonne is working closely with the following industry associations to apply the Laboratory's skills, facilities, and core capabilities:

• Chemicals: Council for Chemical Research

• Refining: American Petroleum Institute

• Forest products: American Forest and Paper Association

• Steel: American Iron and Steel Institute

• Aluminum: Aluminum Association, SECAT LLC

• Metal casting: Cast Metal Coalition

• Glass: Glass Manufacturers Industry Council

In other work, an Argonne initiative aims to develop less costly biotechnological methods of producing valuable products from agricultural materials. See the discussion of Biobased Products in Section IV.A.2.f.

Superconductivity. There is increasing conviction among electric utilities and their suppliers that new technology based on high-temperature superconductivity will provide substantial benefits. This industry support is reflected in projected increases in DOE funding of R&D in the area. Several respected international studies have predicted that global annual sales for all technologies based on high-temperature superconductivity will reach billions of dollars by the year 2020. International competition for these sales will be strong, particularly from Japan and Western Europe.

Argonne is uniquely positioned to develop new technologies based on high-temperature superconductivity. The Laboratory's program of basic science in the field is one of the strongest in the world. Close cooperation continues with the Laboratory's applied superconductivity program, which has produced many notable achievements. Argonne plans to be a major contributor to the development of the second-generation conductor, building on industrial successes already achieved with first-generation powder-in-tube technology. The Laboratory also is contributing to the development of a flywheel incorporating superconducting bearings. Argonne will expand the range of utility applications on which it works, taking advantage particularly of new ideas for fault-current limiters, transmission cables, and motors based on superconductivity. Work in nonutility applications will expand as well, on the basis of innovative ideas in areas such as magnetic separation.

Fossil Fuels and Carbon Management. Among Congress and the presidential administration, there appears to be growing bipartisan support for DOE research related to carbon management. A consortium of major petroleum companies is working with the DOE Office of Fossil Energy to plan major field demonstrations of technologies for the economical sequestration of carbon dioxide. The President's FY 2003 budget request includes additional funding for field-scale testing.

Partnering. Congressional appropriations have continued to reduce funding explicitly available for participation by DOE in industrial partnerships. Argonne's industrial partnerships have been severely constrained by this lack of support.

To maximize the likelihood of establishing effective industrial partnerships in the most promising area of technology, Argonne is seeking opportunities to include other national laboratories and universities in productive strategic collaborations based on the Laboratory's scientific and technical capabilities and its core competencies. The Laboratory has already established a vigorous regional outreach program whose broad goal is to help manufacturers in the Midwest. The Laboratory measures the success of its industrial partnerships by considering the significance and impact of the work accomplished and of the ultimate successful commercialization of new technologies.

c. Transportation Technologies

Situation

The world's transportation system depends critically on petroleum. Oil-derived fuels supply 96% of the energy used to move people and goods. Demand for these fuels continues to grow rapidly, rising by 75% in the United States since the oil crises of the 1970s. Worldwide, the demand for transportation fuels is expected to increase dramatically, especially as developing economies grow. As a result, the world is rapidly approaching the time when a permanent decline in oil production from conventional sources will begin. The Energy Information Administration forecasts that conventional oil production could begin to decline between 2010 and 2040. As the relative price of transportation fuels rises, vehicles with greater energy efficiency will become increasingly important.

The DOE leads two major research programs designed to reduce oil demand by developing vehicles with greater energy efficiency. These programs are the FreedomCAR Partnership (for light-duty vehicles) and the 21st Century Truck Program (for heavy-duty vehicles). Successful development of vehicles that are dramatically more efficient, along with development of alternative fuels, would reduce oil imports, increase energy security, and reduce environmental impacts.

Argonne's Transportation Technology R&D Center is one of DOE's leading research facilities dedicated to addressing the nation's transportation energy problems. Located in the heart of the Midwest, near the nation's manufacturers of automobiles, trucks, and locomotives, the Laboratory works closely with both manufacturers and suppliers to develop cost-effective technologies that improve fuel efficiency and reduce environmental impacts. Argonne maintains a web site that describes the research facilities and capabilities of its Transportation Technologies program (URL: www.transportation.anl.gov).

Vision

Transportation and energy infrastructure will always be critical to U.S. national security. Argonne's Transportation Technology R&D Center will become the premiere provider of needed knowledge about transportation technology and its application, for the nation's industrial, academic, and government research communities.

Goals and Objectives

Argonne's Transportation Technology R&D Center will support the nation's needs for R&D on transportation technology. This goal will be accomplished through basic research, through technology development, and through the creation of partnerships with industry, academia, and other federal or national laboratories that promote energy self-sufficiency and improve energy- and transportation-related technologies serving the national interest.

Specific objectives include the following:

• Work with the FreedomCAR Partnership (which includes the DOE Office of Advanced Automotive Technologies, Ford, General Motors, and DaimlerChrysler) to

- Ensure reliable systems for future fuel cell powertrains, with costs comparable to those of conventional systems (internal combustion engine with automatic transmission) and

- Enable the transition to a hydrogen economy, ensure widespread availability of hydrogen fuels, and retain the functional characteristics of current vehicles.

• Work with DOE and truck engine manufacturers to improve the efficiency and reduce the emissions of advanced diesel technology for use in vehicles of all sizes.

• Develop new technology with a private-sector partner, General Motors Electro-Motive Division, to meet federal locomotive emissions requirements and still achieve high efficiency.

• Work with DOE to develop advanced off-highway and railroad technologies, on the basis of opportunities identified in consultation with industry stakeholders.

Issues and Strategies

Argonne's transportation research, domestic and international, focuses on the following areas where the Laboratory has organized expertise and unique facilities:

• *Vehicle Systems*. New vehicle systems promise to overcome the main limitations of conventional electric vehicles, namely range and recharging rate. Hybrid vehicles typically employ a small combustion engine with a battery or ultracapacitor. The result is the performance of a conventional vehicle but greater efficiency and fewer emissions. Argonne's Advanced Powertrain Test Facility validates DOE-funded components with data on performance and emissions. The Laboratory's vehicle systems models can then simulate actual vehicle systems performance and emissions.

• *Fuel Cells*. Fuel cells convert chemical energy directly into electrical energy, cleanly and efficiently. Fuel-cell-powered vehicles could nearly double the energy efficiency of today's conventional vehicles and reduce emissions by 99%. Argonne has developed a partial-oxidation reformer that converts gasoline to hydrogen-rich gas for use in fuel cells based on polymer electrolyte membranes. The Laboratory's Fuel Cell Test Facility is capable of testing fuel cells up to 50 kW in size. Argonne is also developing solid oxide fuel cells for transportation use.

• *Energy Storage Devices*. In response to stringent environmental regulations, Argonne is developing advanced batteries for electric vehicles. In particular, the Laboratory is working through the U.S. Advanced Battery Consortium to develop commercially viable high-power lithium-ion storage batteries. This work ranges from research on materials for improved anodes and cathodes to development of novel low-cost packaging. Argonne's Analysis and Diagnostics Laboratory performs independent evaluations of batteries developed worldwide.

• *Emissions Control*. By focusing on fuel injector systems and sensors, Argonne plans to develop technologies that simultaneously reduce emissions of particulates and nitrogen oxides from gasoline and diesel engines of all sizes. Until recently, the optically dense regions of the fuel spray from injector systems have been very difficult to image. However, insights from using the world's brightest x-rays, provided by the APS, promise improved understanding of combustion and soot formation, leading to the development of more efficient engines.

• *High-Performance Computing.* Argonne has supported the transportation industry in the design and testing of new concepts for aerodynamics, thermal management, and safety features. Two major efforts are analyzing underhood cooling and crash-worthiness.

• *Recycling*. Obsolete motor vehicles contain plastics, chlorofluorocarbons, rubber, glass, and heavy metals that today are generally not recyclable and must be put into a landfill. Working closely with the auto industry, Argonne is developing economical processes for converting vehicle waste streams into recycled products.

• *Advanced Materials*. Argonne's advanced materials program includes the development of nearly frictionless carbon coatings to reduce the friction and wear caused by sliding and rotating vehicle components. The program also includes the development of new technologies for sensors, rapid prototyping, nondestructive evaluation of ceramic parts, compact heat exchangers, and nanofluids for coolants. Each of these materials technologies promises to improve both the performance and fuel efficiency of vehicles. Use of the APS is expected to assist in the development of catalysts and other new transportation materials.

d. Environmental Treatment Technologies

Separate plans are presented for three areas of environmental treatment technologies at Argonne: (1) EBR-II spent fuel pyroprocessing, (2) radioactive and mixed waste treatment, and (3) decontamination and decommissioning (D&D).

i. EBR-II Spent Fuel Pyroprocessing

Situation

For nearly four decades, research, development, and demonstration associated with liquid metal fast breeder reactors were conducted at EBR-II, located about 40 miles west of Idaho Falls, Idaho; the Enrico Fermi Atomic Power Plant (Fermi-1) in Monroe, Michigan; and the Fast Flux Test Facility at the Hanford Site in Richland, Washington. These activities generated approximately 60 metric tons of sodium-bonded spent nuclear fuel. DOE is now responsible for safe management and disposition of this spent fuel.

Sodium-bonded spent nuclear fuel must be treated differently from other spent fuel because of the presence of metallic sodium (a highly reactive material), metallic uranium and plutonium (also potentially reactive), and, in some cases, highly enriched uranium. Metallic sodium in particular presents challenges for the management and ultimate disposal of spent nuclear fuel, because the element reacts with water to produce explosive hydrogen gas, as well as corrosive sodium hydroxide that is likely to be unacceptable for geologic disposal.

Argonne's pyroprocess for treating metallic spent nuclear fuel uses electrorefining, a type of technology often used by industry to produce pure metals from impure feedstocks. Application of Argonne's pyroprocess has been demonstrated for the stainless-steel-clad uranium alloy fuel and blanket assemblies from EBR-II. A modified process could be used to treat oxide, nitride, and carbide sodium-bonded spent nuclear fuel.

Application of pyroprocessing to EBR-II spent fuel involves several steps. The fuel is first chopped, placed in molten salt, and electrorefined. After electrorefining, the molten salt, fission products, sodium, and transuranics (including plutonium) are removed from the electrorefiner, mixed with the ion exchange agent zeolite, and heated so that the salt becomes sorbed into the zeolite structure. Glass powder is then added to the zeolite mixture and consolidated to produce high-level radioactive waste in the form of a ceramic. The uranium from the electrorefiner is removed, melted, and processed in a furnace to produce low-enrichment or depleted uranium ingots. The stainless steel cladding hulls and the insoluble fission products are melted in a casting furnace to produce high-level radioactive waste in a metallic form.

A three-year demonstration of treating EBR-II spent nuclear fuel was completed in 1999. A subcommittee of the National Research Council judged that the demonstration met all success criteria. DOE then selected pyroprocessing (also known as electrometallurgical treatment) for the complete inventory of EBR-II sodium-bonded fuel, work now under way at Argonne-West.

Vision

Through treatment of EBR-II and other sodium-bonded spent fuel, Argonne will demonstrate that pyroprocessing technology is a cost-effective option that provides a viable approach to managing spent nuclear fuel.

Issues and Strategies

In September 2000, Argonne initiated treatment operations with EBR-II fuel. Processing rates will be increased from the demonstration rates to a total of 600 kilograms in the first year. As funding becomes available for additional staffing, the processing goal for the following year will be 2,000 kilograms of heavy metal. The capacity rate of 5 metric tons per year is to be reached after processing improvements are implemented.

An important issue associated with treatment of EBR-II spent fuel is continued development of the pyroprocess treatment technology in order to achieve the throughput rates required for economical operation. Although the basic technology has been demonstrated, product losses and waste streams should be reduced, new equipment should be produced, and batch size should be optimized. The cost of continued technology development will be a significant fraction of total costs during the first several years of operation.

Waste form development and qualification will extend well into the schedule for treating EBR-II spent fuel, because licensing of the new waste forms for ultimate disposal in a repository requires completion of an extensive behavior characterization database, reflecting both short-term tests and long-term tests with actual radioactive wastes that will extend several more years. Nevertheless, tests with surrogate fission products and limited tests with actual radioactive waste forms have provided sufficient data to establish the viability of the new waste forms.

ii. Radioactive and Mixed Waste Treatment

Situation

Many of DOE’s highest-priority business goals depend directly on the Department’s environmental program, specifically on the objectives of the DOE Office of Environmental Management (DOE-EM). Included in the DOE-EM plan is application of new technologies that have reached various stages of development with support from the DOE-EM Office of Science and Technology.

Argonne has demonstrated significant core capabilities in advanced environmental technologies, built on its broad competencies in nuclear technology and environmental science and technology; its existing nuclear facilities; and its extensive understanding of and experience in resolving complex environmental problems at sites of DOE, the Department of Defense, other federal agencies, and U.S. industry. Integration of capabilities in environmental research, technology development and deployment, comprehensive assessment, and remediation applications is the basis for Argonne’s continuing development of advanced environmental technologies tailored specifically to particular facilities and waste streams for many different types of customers.

Argonne plans to construct the Remote Treatment Facility (RTF) at Argonne-West to provide the infrastructure needed to carry out three missions important to DOE, the state of Idaho, and the national nuclear complex: (1) near-term management of wastes resulting from nuclear research conducted in earlier years at Argonne-West and INEEL, (2) R&D to achieve nuclear energy and national security goals, and (3) R&D to achieve environmental technology goals. Special needs in each of these three areas require that DOE operate facilities dedicated to the development, testing, and implementation of technologies and processes involving the remote handling of highly radioactive materials and the use of intense radiation sources. Argonne will operate the RTF both to meet local waste management needs and to serve as a national user facility for the development and testing of remote technologies. The RTF will augment the existing Hot Fuel Examination Facility (HFEF) at Argonne-West. Development of the RTF will include an addition to the present HFEF and integration of existing HFEF support capabilities, such as analytic chemistry laboratories, into RTF operations.

The 1995 settlement agreement and consent order in the action "United States v. Batt" (the Batt Agreement) requires that DOE provide the treatment and preparation needed for all transuranic waste located at INEEL and ship the waste out of the state of Idaho by 2018. To meet near-term commitments specified in the settlement agreement, the RTF must be operational by 2006. During FY 2001, DOE approved the mission need statement for the RTF.

Vision

Argonne will advance understanding of environmental problems and will develop technologies that allow cost-effective remediation or prevention of those problems for nuclear waste, mixed waste, and other contaminants.

Objectives

Argonne's work on advanced environmental technologies has the following central objectives:

- Develop technologies and facilities for treating mixed waste and nuclear materials.
- Develop superior waste forms and methods of testing and validating techniques for predicting performance.
- Develop innovative environmental technologies that exploit the state of the art in separation science, chemical interactions, and advanced materials.
- Integrate scientific research with field engineering experience and methodologies in order to develop cost-effective solutions to environmental problems.

These Argonne objectives clearly help to address two "gaps" identified in DOE's September 2000 R&D portfolio analysis for its Environmental Quality mission area: (1) dispose of transuranic, low-level, mixed low-level, and hazardous waste (gap number 8) and (2) manage nuclear material (gap number 6).

Issues and Strategies

Development of advanced technologies for mixed waste treatment is a logical extension of Argonne's broad background in reactor technology. In mixed waste treatment, Argonne plans to continue to specialize in remote-handling operations, transuranics, waste form development, environmental process monitoring, and non-thermal treatment options.

Argonne-West already deals with significant amounts of remotely handled radioactive and mixed wastes, which are stored at its Radioactive Scrap and Waste Facility. These wastes require additional characterization, segregation, treatment, and repackaging.

The RTF will be designed to segregate, characterize, treat, and repackage remotely handled materials. The essential features of the RTF are an air atmosphere hot cell with 13 work stations, a hot repair area with access to the hot cell, waste cask handling capabilities, and a cell for nondestructive analysis. Equipment to be installed in the RTF includes a liner disassembly station, an automated waste sorting station, a sodium removal station, an induction furnace, and a waste repackaging station. Direct linkage with the HFEF will be through a cask tunnel. The cask transfer system will be capable of dealing with many types of casks, including the commercial nuclear fuel casks that are licensed for remotely handled transuranic waste. Waste packages that are not compatible with casks will enter the RTF cell through the hot repair area.

Development of stabilized waste forms is very important for solving problems associated with high-level and mixed waste. During the last decade, Argonne has performed a wide range of R&D contributing to waste form development, including long-term and accelerated testing of high-level waste glasses and technical support to the Yucca Mountain Project, development of room-temperature setting of chemically bonded phosphate ceramic waste forms, studies of glass compositional envelopes for DOE-EM, definition of performance specifications for Hanford low-level wastes, and phosphate mineralization of actinides achieved by the measured addition of precipitating anions. Argonne will continue to support DOE programs such as the high-level waste repository and the Waste Isolation Pilot Plant. In addition, technical support will be provided to DOE field offices and to the site contractors at major sites charged with cleanup and waste management, such as Savannah River, Fernald, Rocky Flats, INEEL, and Hanford.

Argonne will continue to support DOE-EM R&D aimed at long-term disposal of waste forms. This research centers around the physics and chemistry of surfaces and interfaces; development of new waste forms for "problem" wastes; and modeling, validation, and performance testing.

iii. D&D

Situation

Decontamination and decommissioning of production and research reactors and nuclear manufacturing facilities represents a major challenge for DOE and the commercial nuclear industry. Problems associated with D&D include safe and effective dismantlement of contaminated and radioactive components; packaging, transportation, and disposal of waste; and recycling and reuse of material.

Argonne is uniquely positioned to assume a leadership role in the development and demonstration of D&D technologies. A number of the technologies already developed or under development at the Laboratory can be applied to D&D, including advanced cutting technologies (such as lasers, water jets, and plasma arcs), effluent control technologies (such as filters for aerosols and dissolved contaminants), instrumentation, decontamination methods (both chemical and mechanical), and risk assessment methods.

Argonne is building its D&D technology program on a strong foundation of extensive experience in nuclear and environmental work, recent success in applying D&D technologies, and valuable strategic partnerships. The Laboratory has experience with the D&D of many types of nuclear facilities, including reactors, hot cells, and facilities containing glove boxes. The most significant of its reactor D&D projects involved the CP-5 Research Reactor and the Experimental Boiling Water Reactor. Argonne also has a long history of developing and deploying both nuclear and nonnuclear technologies, and it has played a leading role in this country's first D&D technology demonstration program at a working D&D site. The CP-5 Large Scale Demonstration and Deployment Project was judged one of DOE's "Top 100 Achievements of the Century." The Laboratory has been instrumental in developing risk-based analyses for recycle and release criteria and for transportation. Its RESRAD (RESidual RADioactivity) family of computer codes is widely used by regulators to aid in evaluating compliance, through estimation of doses and related risks to human health and the environment that result from exposure to radioactivity and chemically contaminated materials. Argonne has also developed cost-engineering models that have been used to validate cost estimates throughout the DOE complex. Argonne is active in several international organizations involved in D&D and has initiated information exchange programs with the International Atomic Energy Agency, Japan, Russia, and Argentina.

Vision

To optimize the cost-effectiveness and safety of D&D operations, Argonne's D&D technology program will continue to advance the development, demonstration, and deployment of cost-saving D&D technologies and to develop and execute analyses of risk, safety, environmental impacts, and costs for DOE, other federal agencies, regulators, and the commercial sector. The program will also continue its contributions to D&D education through training, workshops, and personnel exchanges.

Objectives

The main objectives of Argonne's D&D technology program are the following:

- Provide substantive information on the use and value of D&D technologies for all categories of end users.
- Coordinate the research, development, demonstration, and evaluation of D&D technologies in order to achieve cost-effective D&D for the DOE complex.
- Provide technical services and support in the areas of risk, safety, and cost analysis, as

well as in planning and technology deployment.

- Provide D&D training and participate in informational and educational exchange both domestically and internationally, including support for D&D in the former Soviet Union.

- Work with the DOE Environmental Management Science Program to encourage basic research in areas that will benefit D&D technology.

Issues and Strategies

Key to the development of Argonne's D&D technology program is formation of strategic alliances among national laboratories, utilities, universities, D&D contractors, and technology developers and providers. Argonne will continue to pursue appropriate alliances with nuclear utilities and D&D contractors, as well as with the Nuclear Energy Institute and the Electric Power Research Institute. In all its D&D technology efforts, Argonne is working closely with DOE-Chicago Operations. Internationally, Argonne will take advantage of the Laboratory's strong international research reactor program, which dates back to Argonne's design of research reactors and, more recently, to the design and implementation of proliferation-resistant fuels for research reactors.

A number of external and internal factors will influence the success of Argonne's D&D technology program. External factors include scheduling of D&D by DOE and utilities, effects of utility deregulation, and the availability of low-cost disposal sites for low-level nuclear waste. Internal factors include close integration of the Laboratory's diverse capabilities in technology and advanced technical services. Equally important is the formation of partnerships and strategic alliances with organizations outside the Laboratory.

e. Energy and Environmental Systems

Situation

Long-term energy resources and environmental impacts from energy consumption remain controversial public concerns complicated by economic importance and contradictory public perceptions. Informed decision making in this area requires accurate, clearly presented analyses based on a very wide range of technical information. Federal policy analysis is further complicated because responsibilities relating to energy and the environment are spread widely across federal agencies. No single agency has a mandate to examine the full range of relevant issues.

For decades, Argonne has created technically and economically efficient solutions for energy and environmental problems by applying scientific methods in the development and assessment of new and modified technologies and processes. The Laboratory's successes in this area stem from its capacity to assemble interdisciplinary teams of specialists and to integrate diverse technical resources in order to address difficult problems through focused study and exploitation of unique facilities. A particular Argonne strength is its capability for merging decision analysis, risk assessment, information sciences, and economic evaluations with the engineering specialties and the physical, biological, and social sciences.

Energy and environmental problems create these challenging national needs:

- The rapidly growing complexity of the energy system and related environmental issues necessitate a multidisciplinary, integrated approach to solutions.

- Solutions to environmental problems must be both cost-effective and acceptable to the public.

- The growing information glut facing all decision makers requires the development of better ways to capture, merge, and display critical information.

- Such policy areas as climate change, pollution remediation, and resource management increasingly require global analysis and international coordination.

- There is growing evidence that restructuring of the U.S. electric system requires new approaches to reliability, environmental protection, and preparation for disruptions. At the same time, new environmental regulations require the development and adoption of advanced procedures and technologies.

• The benefits of increasing the production of fossil fuels on U.S. public lands must be balanced against the need to protect environmental quality.

Vision

Argonne will provide national and international leadership in the creation of innovative and cost-effective solutions to energy and environmental problems, through the development of next-generation technologies; through the application of state-of-the-art techniques in assessment, risk analysis, and decision analysis; and through the transfer of those technologies to the private sector and other researchers.

Objectives

Key objectives of Argonne's program in Energy and Environmental Systems include the following:

• To improve the analysis and assessment of advanced energy systems, develop models, methodologies, and techniques that give decision makers more accurate information about the changing structure of the energy system, particularly the electric power system.

• Develop integrated environmental assessments, risk analyses, modeling techniques, and innovative information systems (by using approaches such as advanced visualization, advanced data management techniques, and spatial and geographic information systems) that benefit federal managers, policy makers, and private-sector businesses facing new regulatory requirements.

• Apply these energy and environmental tools, techniques, and methodologies to issues of national concern; transfer the tools to other researchers and to private-sector energy organizations for improved decision making.

• To improve the cleanup and subsequent long-term stewardship of Cold War legacy waste sites, make available more widely — to DOE, federal, and private-sector sites — the benefits of Argonne's unique capabilities in information management; in tools for assessing the changing structure of energy systems; and in methods of site characterization, remediation, and restoration.

• Expand the Laboratory's international activities that address global climate change and environmental protection.

Issues and Strategies

Argonne's strategies for achieving its objectives in Energy and Environmental Systems include the following:

• Take advantage of Argonne's strengths in high-performance computing and multidisciplinary domains to investigate the application of advanced techniques — such as complex adaptive systems analysis and agent-based simulation — and provide better decision making information in the rapidly changing, highly complex, nonlinear arena of energy and environmental policy.

• Combine innovative decision tools with field techniques to create applied environmental methodologies that are more effective. For example, tailor more cost-effective approaches to site cleanup and long-term stewardship through better site sampling strategies, better monitoring methodologies, and more flexible decision-making practices based on rapid acquisition and evaluation of accurate field data.

• Address emerging technical issues associated with long-term environmental stewardship at DOE and other federal facilities, especially sites requiring extensive cleanup. (See discussion of the initiative Science and Technology for Environmental Stewardship at the end of this area plan.)

• Collaborate with urban community groups to increase the stock of energy-efficient buildings, including housing and schools; to return abandoned sites to use; and to design and implement next-generation modes of urban transportation. These efforts will include integration of Argonne techniques, technologies, tools, and training to foster the creation of more high-wage jobs, to ease urban blight, and to support the renovation of urban infrastructure.

- Explore additional opportunities to apply the Laboratory's special capabilities beyond DOE, to benefit the Departments of Defense, Agriculture, and the Interior; the Nuclear Regulatory Commission; other federal agencies; state and municipal governments; nongovernmental organizations; and the private sector.
- Expand activities with international organizations and appropriate foreign governmental organizations involving the analysis of international issues concerning energy and environmental systems — including global electric system restructuring, transnational energy system interconnections, global climate change, sustainable development, hazardous waste generation, and ecosystem management.

In summary, Argonne has considerable strength in most scientific and technical areas related to energy and the environment. The Laboratory is well organized to integrate its multidisciplinary capabilities in research, development, and demonstration of new technologies. Recognition of these capabilities has allowed Argonne to develop solutions to a wide variety of real-world problems and to strengthen its relationships with sponsors further. Current challenges include developing innovative methodologies for analyzing energy and environmental problems (such as global climate change and restructuring of the electricity market) that cannot be addressed adequately with conventional techniques; identifying appropriate opportunities for beneficial external collaboration; and extending the breadth and depth of the Laboratory's capabilities.

Initiative: Science and Technology for Environmental Stewardship

The DOE R&D portfolio analysis for the Environmental Quality mission area in September 2000 identified long-term environmental stewardship as one of four highest-priority technical "gap" categories. In response to this need, Argonne proposes a program of research, development, and analysis to address emerging technical issues associated with the environmental stewardship of lands and facilities for which DOE and other federal agencies are responsible.

The concept of environmental stewardship encompasses the mechanisms — physical and institutional controls, information management, environmental monitoring, risk assessment, and other means — needed to ensure, in both the short term and the long term, protection of people and the environment. Government is responsible for stewardship of the lands it manages and for the environmental consequences of its activities. Planning for effective stewardship includes evaluating impacts from the use of rights-of-way on federal lands (such as the Trans-Alaska Pipeline system); assessing the effects of extracting energy and other resources; and developing effective methods of managing residual contamination left following cleanups at government facilities.

This initiative in Science and Technology for Environmental Stewardship takes advantage of Argonne's substantial capabilities and experience in characterization, in analysis and engineering for processes and systems, and in integrated management, including risk assessment. The initiative will emphasize (1) decision making related to risk to human health and ecosystems and (2) monitoring to obtain feedback for updating previous decisions. Such risk assessment requires integration of results from multiple analyses, models, and monitoring. Associated decision making processes often involve disparate stewards, regulators, and the public. Informed decision making depends critically on effective integration and dissemination of relevant information. To create an improved technical basis for stewardship, the Laboratory will investigate the deployment of technologies and approaches it has developed by using advanced techniques of computing and communications.

Resources that can be applied beneficially to this initiative are described in Table IV.7. Funding will be sought initially from DOE-EM (EW, EX); Environment, Safety, and Health (HC); and Science (KP-12, KP-13).

Table IV.7 Science and Technology for Environmental Stewardship ($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	9.3	9.7	10.0	13.0	15.0	17.0	19.0
Capital Equipment	0.2	0.3	0.4	0.5	0.5	0.5	0.5
Construction	-	-	-	-	-	-	-
Total	9.5	10.0	10.4	13.5	15.5	17.5	19.5
Direct Personnel	28.0	30.0	32.0	39.0	40.0	41.0	42.0

f. Biotechnology

Situation

Biotechnology research at Argonne is a multidisciplinary, cross-cutting activity that integrates a variety of disciplines and unique research facilities. The Laboratory is one of DOE's leading resources for developing the technologies of biological microchips and biobased chemicals. Key elements of the Laboratory's program are sponsored by DOE, the Department of Defense, and private-sector industrial collaborators. Near-term plans include further strengthening of capabilities in biocatalytic and downstream processing, in bioinformatics, and in the development of automated systems for gene cloning and expression.

Objectives

Key objectives of Argonne's biotechnology program include the following:

- Development of biological microchips (biochips) for the detection of mutations in human genes and identification of viruses, bacteria, and bacterial toxins
- Evaluation of biochemicals for control of cellular malignancies
- Development of advanced emergency resuscitation technologies, improved artificial intelligence for medical diagnostics, and new prosthetic materials and coatings
- Development of industrial processes based on environmentally friendly, biologically based chemicals and solvents
- Development of technologies to monitor, remove, detoxify, and recover heavy metals, organic compounds, and bacteria in the environment

Issues and Strategies

In addition to national security, Argonne's programs in biotechnology focus on three promising areas having high national priority:

- *Medical Applications.* Programs emphasize development of advanced biochips for analyzing genetic information, studying cancer and biochemicals to guide pharmaceutical development, and developing advanced devices and procedures for emergency resuscitation.
- *Industrial Processes.* Programs include the development of environmentally friendly "green solvents" and biobased chemical production processes (e.g., the use of corn as feedstock for producing chemicals such as ethyl lactate and succinic acid).
- *Environmental Protection.* Programs include investigation of environmentally acceptable methods for treating microbial corrosion in pipelines; field demonstrations of phytoremediation methods; and development of photocatalysts for the removal, detoxification, and recovery of heavy metals and organic compounds in aqueous waste streams.

Initiative: Biochips and DNA

Argonne's established biochip program is invigorated by the continuing rapid emergence of novel potential applications for biochip technology, particularly applications that involve DNA decoding and imply valuable opportunities for spin-off initiatives. These spin-offs are currently focused on four key areas:

- Analysis of changes (mutations) in genetic makeup
- Identification of bacteria, viruses, and their products
- Detection and rapid analysis of biological threat agents

- Development of phylogenic chips to improve analytic sensitivity

Argonne's Biochips and DNA initiative aims to develop and apply both generic and customized biochips in the above areas. Generic biochips are useful for reading unknown sequences, and customized biochips are used to study phenomena such as gene polymorphism (which may be associated with susceptibility to various autoimmune diseases). A recent thrust is the collaborative development of a three-dimensional biochip that offers major advantages over currently available two-dimensional designs. The resources required for this initiative are summarized in Table IV.8. The funding increase for FY 2003 is sought from DOE, other federal agencies, and the private sector.

Table IV.8 Biochips and DNA
($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	4.0	4.4	4.4	4.4	4.4	4.4	4.4
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	4.0	4.4	4.4	4.4	4.4	4.4	4.4
Direct Personnel	10.0	11.0	11.0	11.0	11.0	11.0	11.0

Initiative: Biobased Products

Argonne's biobased products program, like the Laboratory's biochip technology program, is an established activity that often spins off initiatives as novel potential applications are identified. Current components of the Biobased Products initiative range from the development of additional uses for corn as a chemical feedstock to the development of advanced membrane processes that lower the cost of downstream processing and purification. Nanoscience and structural biology are being applied to address fundamental issues in biocatalysis and processing, particularly issues that affect product cost. Resources required for this initiative are summarized in Table IV.9. Funding is sought from DOE-Energy Efficiency (ED), DOE-Fossil Energy (AA), other federal agencies, and industrial partners.

Table IV.9 Biobased Products
($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	2.5	2.5	3.0	3.0	3.0	3.0	3.0
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	2.5	2.5	3.0	3.0	3.0	3.0	3.0
Direct Personnel	10.0	10.0	12.0	12.0	12.0	12.0	12.0

3. National Security

As stated by Secretary Abraham, national security is the overarching mission of DOE. It is also one of the four traditional underlying mission areas of the Department.

a. Nuclear Nonproliferation and Arms Control

Situation

Argonne's current nonproliferation work aims to reduce the threat to U.S. national security posed by nuclear, chemical, and biological weapons. At the end of the Cold War, the principal threat to U.S. national security changed from large-scale nuclear war to asymmetric conflicts and terrorist activities by subnational groups. The Laboratory's earlier focus on technical means to verify treaty compliance has shifted toward developing ways to limit the spread of weapons of mass destruction.

Among the most pressing problems facing the United States is the breakdown of systems for controlling nuclear materials in Russia and the independent states that resulted from the dissolution of the former Soviet Union (FSU). The United States is one of several countries providing technical assistance to these nations to help improve their systems for control of nuclear materials.

Argonne's nonproliferation and arms control program, with an annual budget totaling approximately $20 million, includes several significant components:

- The Reduced Enrichment for Research and Test Reactors (RERTR) program, which develops new fuels, targets, and analysis methods to enable research reactors throughout the world to replace highly enriched uranium in their fuel and targets with low-enrichment uranium.

• The Material Protection Control and Accounting (MPC&A) program, which assists nuclear facilities in Russia and the countries of the FSU. Assistance is offered through surveying the current status of protection and accounting for nuclear materials, making recommendations for improvements, and coordinating upgrade plans and their implementation. This program includes training courses offered both at Argonne and abroad, to enable foreign specialists to effectively utilize new security and accounting systems.

• The Verification Technology program, which develops sensitive and selective instruments to detect radiation and chemical and biological effluents that might indicate clandestine proliferation.

• The Nuclear Export Control program, which provides technical assistance to the National Nuclear Security Administration (NNSA). The assistance includes (1) assessments of proliferation risk associated with proposed exports of nuclear and nuclear-related dual-use material, equipment, and technologies and (2) establishment and improvement of effective systems of export control in Russia and countries of the FSU.

• Packaging and storage of nuclear materials from the BN-350 breeder reactor in Kazakhstan, which implements U.S. nonproliferation goals by improving the security of the plutonium in the BN-350 spent fuel and blanket assemblies.

• Irreversible shutdown of the BN-350 breeder reactor in Kazakhstan, which serves U.S. nonproliferation goals by ensuring that the reactor can never again produce nuclear materials suitable for weapons. This program utilizes a unique organizational approach in which integrated design teams are established between various Kazakhstan organizations and Argonne to resolve issues that arise.

• The joint U.S.-Russian materials disposition program, which targets the disposal of excess weapons plutonium by reactor irradiation. As part of this effort, the BN-600 fast reactor is being converted to a configuration that burns plutonium.

• The Highly Enriched Uranium Transparency Program, which monitors the blending down of highly enriched uranium from dismantled Russian nuclear weapons to produce low-enrichment uranium for eventual use as commercial reactor fuel in the United States, thereby encouraging compliance with international treaty obligations and reducing the threat of nuclear proliferation.

• The Initiatives for Proliferation Prevention (IPP) and the Nuclear Cities Initiative (NCI), which engage former nuclear, biological, and chemical weapons workers in Russia, Ukraine, and Kazakhstan in development of new civilian, peaceful occupations, in collaboration with U.S. companies working under cooperative R&D agreements with Argonne scientists. (The NCI only helps workers in Russian closed cities.)

Mission

By exploiting the technical and analytical expertise of Laboratory staff and the Laboratory's facilities for physical and biological research, Argonne supports the efforts of federal agencies to reduce threats to national security that would result from the proliferation or use of weapons of mass destruction. In addition, Argonne helps to implement associated U.S. policy initiatives.

Issues and Strategies

Argonne plans to integrate and increase its support for nuclear nonproliferation initiatives, particularly by exploiting the Laboratory's unique expertise in nuclear and sensor technologies. The RERTR activities will involve extensive cooperation with Russia and more than 25 other countries. Many international research reactors are today fueled with highly enriched uranium and cannot be converted to low-enrichment fuel by using current technologies. The Laboratory plans to develop the required new nuclear fuels. In addition, the Laboratory will develop new targets and chemical processing to produce molybdenum-99, an important medical radioisotope, by using low-enrichment uranium instead of highly enriched uranium. The Laboratory also plans to develop new instruments to detect the presence of chemical and biological weapons. Argonne expertise will be used to enhance the security of nuclear materials at additional sites in the FSU and also to reduce the availability of weapons-usable materials by reducing stockpiles of highly enriched uranium. Other activities will focus on developing spin-off projects related to the Laboratory's established MPC&A and training programs in Russia and the countries of the FSU. Laboratory technical staff will continue to support NNSA efforts to promote effective nuclear export controls. The IPP program will be extended to engage former biological and chemical weapon workers in the FSU. The NCI program will help place former nuclear weapon scientists in commercial projects at the Sarov Open Computing Center. On the basis of its expertise in nuclear fuel management, the Laboratory has a technical leadership role in packaging and storing spent nuclear fuel at the BN-350 fast reactor in Kazakhstan to improve the material's proliferation resistance. In addition, Argonne was selected to serve as one of two lead laboratories for a proposed project to assist Russia with the design and construction of a dry storage facility for fuel awaiting reprocessing at Mayak. The initiative Nonproliferation Technologies, discussed below, proposes significant expansion of Argonne's work on the development, demonstration, and deployment of nuclear material safeguard technologies.

Recent terrorist attacks have underlined the need for increased attention to national nuclear security and homeland defense. Weapons of mass destruction and the materials that are key to their production must continue to receive attention, and the need to address nontraditional challenges has risen to unprecedented importance. Systems originally designed to address more traditional threats must evolve in order to plan adequately for and respond to new potential targets, different modes of delivery, different weapons, and different consequences, including functional defeat of critical economic infrastructure and processes. To strengthen the prevention of domestic and international nuclear events, Argonne proposes five new initiatives:

1. Nonproliferation Technologies
2. Nuclear Fuel Cycle Technology Applications
3. Training for Specialists in Nuclear Material Protection and Law Enforcement
4. International Nuclear Safety and Cooperation
5. Integrated Research Reactor Safety Enhancement Program

Initiative: Nonproliferation Technologies

Argonne proposes significant expansion of its activities related to the development, demonstration, and deployment of nuclear material safeguard and process monitoring technology. For NNSA and DOE-EM, the Laboratory's established sponsors in these areas, this initiative addresses nondestructive assay of materials, monitoring and surveillance systems, and advanced software products. The Laboratory will also leverage its expertise in special nuclear material handling and physics, along with its associated facilities and materials, to conduct process testing of related technologies developed at Argonne and elsewhere in the DOE complex. Technology development initiatives will be tied to the Laboratory's unique physical resources — including its nuclear materials and remote handling facilities — and ongoing nuclear technology projects. These broadly applicable technologies could also serve DOE-Civilian Radioactive Waste Management and the Department of Defense, as well as other federal agencies.

This Nonproliferation Technologies initiative obtains strong leverage from core Argonne programs in spent nuclear fuel treatment, nuclear waste, nonproliferation, facility operations, nuclear safety modeling, and other areas.

Funding for this initiative will be sought from NNSA (NN), DOE-EM (EW); and the Department of Defense. See Table IV.10.

Table IV.10 Nonproliferation Technologies
($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	1.0	2.5	3.5	3.5	3.5	3.5	3.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	1.0	2.5	3.5	3.5	3.5	3.5	3.5
Direct Personnel	2.5	5.0	7.5	7.5	7.5	7.5	7.5

Initiative: Nuclear Fuel Cycle Technology Applications

Argonne is a leader in the technology of the nuclear fuel cycle. This initiative proposes application of Laboratory expertise and facilities to reducing the likelihood of diversion of nuclear materials throughout the nuclear fuel cycle, to identifying materials detected in illicit commerce, and to characterizing materials that might be encountered in a nuclear incident.

Methodology for Nuclear Fuel Cycle Observability and Transparency

Observability and transparency are critical objectives in improving the proliferation resistance of existing and future nuclear fuel cycles. Advanced nuclear fuel cycles must be designed to maximize those attributes for the facilities of all nonweapons member states of the IAEA. Initially designing fuel cycle processes and operations to be more observable and transparent reduces the potential for undetected proliferation. A formal methodology for implementing observability and transparency facilitates integration of attributes inherent in plant operation with advanced information and unattended-monitoring technologies. Such integration will achieve the goal of timely verification that only declared operations are being conducted within declared facilities. Such an advanced methodology combines positive verification (i.e., material accountancy) with negative verification (i.e., operations accountancy) to increase the effectiveness of safeguards.

Nuclear Material Attribution

The ability to determine (1) where nuclear materials originated, (2) the capabilities by which they were produced, and (3) the ways in which they might be used is important for interdicting illicit commerce in nuclear materials and for determining the source of nuclear materials obtained by terrorists. Argonne proposes to apply its expertise in nuclear fuel cycles to these three tasks as an expansion of its current work on materials attribution for homeland defense.

Nuclear Material Characterization

Emergency response and mitigation in response to a terrorist attack involving a radiological dispersion device or a crude nuclear device require knowledge of the character of the materials involved and the phenomenology of the device. Argonne proposes to apply its expertise to planning for the characterization of materials produced from such a device (e.g., by understanding the materials' signatures), identifying possible pathways to communities and the environment, and developing means of mitigating the impacts.

Resources for this initiative will be sought from DOE-Defense Nuclear Nonproliferation (NN), the Department of Defense, and other agencies involved in homeland defense. See Table IV.11.

Table IV.11 Nuclear Fuel Cycle Technology Applications ($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	1.2	2.0	2.5	2.5	2.5	2.5	2.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	1.2	2.0	2.5	2.5	2.5	2.5	2.5
Direct Personnel	5.0	9.0	11.5	11.5	11.5	11.5	11.5

Initiative: Training for Specialists in Nuclear Material Protection and Law Enforcement

For several years Argonne has supported the MPC&A program of NNSA by providing training to nuclear security personnel from Russia and the countries of the FSU. This training, conducted at the MPC&A Training Facility at Argonne-West, teaches the latest security concepts and gives students hands-on experience in operating electronic and computerized security systems. In coming years, Argonne will offer to expand the number of classes conducted and thereby enable NNSA to accelerate completion of its MPC&A projects. In addition, the Laboratory will offer its security training facility and expertise to help law enforcement officials meet their homeland security responsibilities. The Laboratory is currently discussing with local law enforcement officials their training needs related to access control for courts, public buildings, and airports.

In addition to offering security experts for foreign projects, Argonne stands ready to provide experts for surveys in support of homeland security.

Resources required are summarized in Table IV.12. Funding will be sought from DOE-Defense Nuclear Nonproliferation (NN).

Table IV.12 Training for Specialists in Nuclear Material Protection and Law Enforcement
($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	2.0	2.5	3.0	3.5	3.5	3.5	3.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	2.0	2.5	3.0	3.5	3.5	3.5	3.5
Direct Personnel	4.0	5.0	6.0	6.5	6.5	6.5	6.5

Initiative: International Nuclear Safety and Cooperation

Argonne's ongoing Soviet-Designed Reactor Safety Program, which assesses the safety of Soviet-designed power reactors, has demonstrated the need for continued U.S. engagement with less developed countries seeking peaceful use of nuclear technologies. Moreover, the ongoing program has revealed important nuclear safety and security issues that extend beyond power reactors. Therefore, the Laboratory proposes to expand its current program to collaborate with countries wishing to assess and address such issues throughout the life cycle of nuclear material. The focus of the expanded program will be assessments of the greatest risks facing nuclear fuel production, transportation, power production, and waste handling activities within a country. Risks considered would include both internal and external threats, whether accidental or intentional, and assessments would recognize the unique circumstances of particular facilities, such as their locations with respect to population centers and the adequacy of local infrastructures to monitor and control nuclear operations. Building on Argonne's safety assessment experience in the FSU, the expanded program would make risk-based recommendations to the countries assessed and to the NNSA about ways to minimize the vulnerabilities of facilities. The new program would include collaborative training, coordinated between Argonne and the IAEA, to transfer safety assessment technology to the participating countries and to link those countries into the network of international nuclear safety centers to improve communication on nuclear safety.

The International Nuclear Safety and Cooperation program will complement the Integrated Research Reactor Safety Enhancement Program (IRRSEP) proposed below, which will specifically address safety and security issues facing research reactors throughout the world. Countries wanting to improve the safety of their research reactors would also benefit from a comprehensive, integrated assessment of other nuclear risks that they face. Such countries could, for example, be encouraged to shut down outdated research reactors if the United States offered training in health physics or emergency preparedness that helped them manage other nuclear operations.

Resource requirements are given in Table IV.13. NNSA funding (AF-15-30) would be supplemented by funding from the U.S. Agency for International Development and from the Nonproliferation and Disarmament Fund.

Table IV.13 International Nuclear Safety and Cooperation ($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	0.6	3.0	5.0	4.0	3.0	3.0	3.0
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	0.6	3.0	5.0	4.0	3.0	3.0	3.0
Direct Personnel	2.0	6.0	7.0	6.0	5.0	5.0	5.0

Initiative: Integrated Research Reactor Safety Enhancement Program

Argonne proposes to significantly expand its work in the area of cooperation and safety enhancement for international research reactors. Research reactors represent a unique safety and security risk for less developed countries. An integrated approach to addressing these risks — based on Argonne's experience in work with research reactors, international safety networks, fuels, and decommissioning — can offer NNSA a more powerful way to improve research reactor safety. By leveraging existing safety infrastructures, the Laboratory can approach facilities of concern in a cooperative manner, assess vulnerabilities, and provide substantial assistance in the areas of fuel characterization, stabilization, and disposition; safety and security upgrades; safety infrastructure development; and emergency preparedness.

Argonne has a long history of working with the owners and operators of foreign reactors and their support organizations to assess and improve nuclear safety. Establishment of networked international nuclear safety centers will continue to provide valuable liaisons with the nuclear communities in the countries of the FSU and elsewhere in the world. This network can provide the framework for reducing research reactor risk and can offer valuable support in areas such as emergency response and health physics training. Many research reactor facilities worldwide suffer from poor quality assurance programs, lack of trained personnel, insufficient safety reviews, and limited regulatory oversight. Working in parallel with the new International Nuclear Safety and Cooperation program proposed above, the IRRSEP can address both broader infrastructure issues and specific facility issues.

Synergies with existing Argonne work for the RERTR program and for material protection programs will be exploited to provide maximum benefit to NNSA. Cooperation with the IAEA and the U.S. Nuclear Regulatory Commission will further enhance the program's effectiveness.

Resource requirements are given in Table IV.14. NNSA funding (NN-30) may be supplemented with funds from the U.S. Agency for International Development and from the Nonproliferation and Disarmament Fund.

Table IV.14 Integrated Research Reactor Safety Enhancement Program ($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	1.0	3.0	5.0	7.5	7.5	7.5	7.5
Capital Equipment	-	-	-	-	-	-	-
Construction	-	-	-	-	-	-	-
Total	1.0	3.0	5.0	7.5	7.5	7.5	7.5
Direct Personnel	4.0	8.0	12.0	15.0	15.0	15.0	15.0

b. Infrastructure Assurance and Counterterrorism

Situation

Argonne's work on infrastructure assurance and counterterrorism aims to assure the security and reliability of critical U.S. infrastructures — and the safety of associated populations — that are threatened by disruptions resulting from natural events, accidents, or deliberate acts such as terrorist attacks. This work addresses cyber security and technologies, as well as capabilities for detecting, combating, and recovering from chemical, biological, and nuclear terrorism (a growing national security concern addressed in the preceding Nuclear Nonproliferation and Arms Control area plan, Section IV.A.3.a). Work in these areas of homeland security directly supports DOE's overarching national security mission.

The Laboratory's work on infrastructure assurance and counterterrorism draws on expertise, knowledge, technologies, and specialized research facilities developed over decades for other purposes. By leveraging the Laboratory's core science and technology competencies, this work responds to the shifting challenges facing the nation. These challenges are complicated by changes in threat profiles, weapons, targets, attackers, and motivations.

Argonne's infrastructure assurance and counterterrorism programs have annual budgets totaling approximately $12 million. Significant components of these programs include the following:

- The Vulnerability Assessment program evaluates the safety and security of critical infrastructure by considering physical security, operations security, cyber security, and infrastructure interdependencies. The program includes comprehensive assessments and rapid surveys.
- The Energy Infrastructure Interdependencies program evaluates the interdependencies among various types of infrastructures (e.g., between electric power and natural gas or between electric power and telecommunications); the potential for cascading impacts resulting from disruptions to one or more types of infrastructures; better methods of detecting events affected by infrastructure interdependency; and improved technologies and procedures for preventing, responding to, and recovering from such events.
- The Infrastructure Outreach program increases the awareness of infrastructure owners and operators concerning security issues. This program also promotes sharing of best practices and lessons learned in infrastructure assurance.
- The Community Critical Infrastructure Protection program, in collaboration with community emergency planners and local utilities, develops plans and procedures that municipalities can use to prevent, respond to, and recover from major disruptions to energy infrastructure (e.g., that for electric power or natural gas).
- The Interior Infrastructure Protection for Chemical/Biological Attacks program demonstrates technologies for mitigating impacts from chemical or biological attacks on interior infrastructure deemed to be at above-average risk, such as subways, airports, and public buildings.

In addition to the programs described above, the Laboratory maintains the following significant capabilities and facilities for addressing potential chemical and biological threats:

- Instruments for detecting potential chemical or biological threats in air, water, and soil, whether dispersed over kilometers or hidden in caches.
- Facilities for evaluating the effectiveness of chemical and biological monitoring methods, at both laboratory scale and field scale.
- Capabilities for determining health and environmental risk from the dispersion of chemical, biological, and nuclear weapons.
- Capabilities for evaluating the effects of agents on materials and for developing protective materials and methods of decontamination.
- Laboratories and expertise for developing prophylactic drugs and vaccines based on structural analyses of biomolecules.
- Fast-response systems for protecting first responders, decreasing exposure times, and reducing risk.
- The capability to conduct laboratory and field analyses enabling attribution of chemical or biological attacks.
- The Electron Microscopy Center, which provides high-resolution scanning electron microscopes able to examine and characterize the nanoscale embodiments likely to be used in chemical and biological detectors.
- The Multi-Bay Robotics Laboratory, which can develop robotic manipulator systems for remote work in unstructured hazardous environments.
- The Mobile Laboratory for Chemical Agent Detection, which is used to characterize chemical agent contamination in U.S. Army buildings. Samples can be analyzed on-site for

rapid turnaround, and the facility can confirm decontamination after cleanup operations.

- The Dilute Chemical Agent Facility, which is approved by the U.S. Army to Level 2 and is certified to accept agents such as soman, sarin, and lewisite. The facility is equipped for development of analytical methods, detector testing, development of decontamination technologies, and validation of transport models. This facility currently serves as an emergency response laboratory for the Environmental Protection Agency.

Other Argonne facilities also provide significant R&D capabilities for addressing potential chemical and biological threats. These include the APS and the associated Structural Biology Center and Midwest Center for Structural Genomics. Though most of the Argonne capabilities and facilities identified here were not specifically established for R&D related to chemical and biological counterterrorism, they nevertheless are significant resources for addressing currently anticipated threats.

Mission

By leveraging Argonne expertise and facilities, both physical and computational, support DOE's overarching national security mission and the complementary efforts of other federal agencies to ensure the security and reliability of our nation's critical infrastructure and reduce threats from weapons of mass destruction.

Issues and Strategy

In the area of infrastructure assurance and counterterrorism, Argonne supports the development of technologies and strategies that improve detection, mitigation, response, and recovery. As described below, the Laboratory plans to expand its work on infrastructure vulnerability and risk assessment, energy systems analysis, analysis of infrastructure interdependencies, emergency preparedness, consequence management, and protection from chemical and biological threats. These activities have been given high priority by the Office of Homeland Security and the White House Office of Science and Technology Policy, and they are cornerstones of DOE's long-term R&D program on critical infrastructure protection.

In the area of counterterrorism, Argonne continues to expand research related to chemical and biological threat analysis, vulnerability assessment, detection and speciation, and incident response and attribution. These activities are based on Laboratory competencies that include (1) molecular biology, (2) structural analysis, (3) radiation chemistry and photochemistry, (4) catalysis and electrochemistry, and (5) chemical and biological decontamination. For example, a microchip-type sensor that employs methods for isolating and labeling RNA (ribonucleic acid) is being evaluated as part of a comparative study sponsored by the Defense Threat Reduction Agency. The Laboratory is also developing other detection methodologies that rely on biomolecular recognition, antibody pairing, or molecular fluorescence. Further current research focuses on ozone-based decontamination systems, aerosol monitoring, and risks associated with chemical warfare agents. During the coming year, Argonne will submit new threat reduction initiatives to DOE and other concerned public agencies. These initiatives are based on both Laboratory expertise and facilities such as the APS, the Structural Biology Center, and the Midwest Center for Structural Genomics.

Initiative: Infrastructure Assurance and Counterterrorism

Argonne proposes to expand its current research, development, and analysis activities in the area of critical infrastructure assurance and counterterrorism. The goal of this work for DOE and other federal agencies is to develop and apply innovative technologies, methodologies, models, and simulations that (1) will better protect critical U.S. infrastructure (including cyber-based information systems) and associated populations from disruption and (2) where disruptions do occur, will improve detection, mitigation of effects, response, and recovery. The Laboratory's capabilities are particularly relevant to the infrastructures for energy (electric power, oil, and natural gas), transportation, agriculture, water supply, information and communications, and emergency services.

This initiative responds to the executive order establishing the Office of Homeland Security and the *Executive Order on Critical Infrastructure Protection in the Information Age*, which outlines key elements of U.S. policy. The initiative is also consistent with the strategic thrust of DOE's Office of Energy Assurance, which was established in December 2001 to serve as the focus for DOE's activities in energy infrastructure assurance. Under these executive orders, DOE is the lead federal agency for assuring the continuity and viability of the nation's critical energy infrastructures.

Argonne's long history of work related to infrastructure assurance and counterterrorism — reinforced by more intensive work over the past five years for the DOE Office of Energy Assurance, the Critical Infrastructure Assurance Office, the Department of Defense, and other government organizations — provides the foundation for this initiative. The Laboratory will expand its work in the areas of vulnerability and risk assessment, energy and water systems analysis, information management, infrastructure interdependencies analysis, modeling and simulation of agent-based and complex adaptive systems, decontamination and remediation, and emergency preparedness and consequence management.

Improved technologies and capabilities are needed in all these areas to address the unprecedented range of physical and cyber threats to critical U.S. infrastructure from natural causes, accidents, and deliberate acts like the terrorist attacks on the World Trade Center and Pentagon. Argonne will particularly emphasize development of methodologies and tools for analyzing the new vulnerabilities that have arisen because various components of the nation's infrastructure have become increasingly complex, automated, physically interconnected, and logically interdependent. The White House Office of Science and Technology Policy has given high priority to research on interdependent infrastructure, and that research is a cornerstone of DOE's long-term program on critical infrastructure protection.

Argonne will continue to enhance its collaboration with other national laboratories as it conducts vulnerability surveys and assessments and develops cost-effective solutions to infrastructure assurance and counterterrorism problems. In the area of chemical and biological threats, the Laboratory is currently leading multilaboratory teams of experts in modeling and analyzing infrastructure interdependencies and protecting civilian interior infrastructures (such as subway systems, airports, and public buildings) deemed to be at above-average risk.

Resources required for this initiative are summarized in Table IV.15. Funding will be sought from the DOE Office of Energy Assurance (GD-05), the NNSA Office of Defense Nuclear Nonproliferation (NN-20), other DOE program offices, and other federal agencies.

Table IV.15 Infrastructure Assurance and Counterterrorism ($ in millions BA, personnel in FTE)

	FY02	FY03	FY04	FY05	FY06	FY07	FY08
Costs							
Operating	12.0	15.0	15.0	15.0	15.0	15.0	15.0
Capital Equipment	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Construction	-	-	-	-	-	-	-
Total	12.1	15.1	15.1	15.1	15.1	15.1	15.1
Direct Personnel	60.0	75.0	75.0	75.0	75.0	75.0	75.0

4. Collaborative R&D Partnerships

Situation

Over the past decade, Argonne's technology transfer program has reinforced the Laboratory's reputation as a reliable, productive partner for industry. The R&D work conducted by the Laboratory in partnership with industry contributes strongly to DOE's strategic goals within the Department's four mission areas.

As part of the Laboratory's focus on strengthening ties with the University of Chicago, operator of Argonne, scientists are pursuing joint research projects and other forms of collaboration. In addition, the technology transfer offices at the Laboratory and the university have begun collaborating in the evaluation and licensing of Laboratory-generated intellectual property. The university brings valuable additional insight to this activity, particularly in the areas of growing research collaboration.

Mission and Vision

The mission and vision of Argonne's technology transfer program include five elements:

- License valuable intellectual property to enhance U.S. economic productivity, while providing a source of revenue for Laboratory use in compliance with the terms of the contract between DOE and the University of Chicago for the management and operation of Argonne.
- Enhance Argonne's R&D programs and increase their funding through interactions with non-DOE government entities and with private institutions, including industry and academia.
- Enhance the worldwide competitiveness of U.S. industry through cost-shared and reimbursable R&D performed by the Laboratory.
- Foster utilization of Argonne's R&D.
- Deliver and leverage a technology transfer program — including policies, processes, and results — that increases returns to Argonne and significantly contributes to the Laboratory's fulfillment of its mission and strategic goals. To this end, (1) improve Argonne's technology transfer policies and processes and (2) increase programmatic and stakeholder satisfaction with the technology transfer program and the associated construction, delivery, and execution of technology transfer solutions.

Issues and Strategies

Numerous cooperative R&D agreements (CRADAs) are supported through Laboratory programmatic activities, and Argonne is increasingly using work-for-others contracts for industrial agreements. Full funds-in CRADAs are also used to advantage to develop cooperative research partnerships, when DOE funding for Laboratory efforts is not available. Argonne continues to increase the precommercial R&D that it performs for private industry.

For further information about technology transfer at Argonne, see Supplement 2.

B. Laboratory Directed R&D Program

Laboratory Directed Research and Development (LDRD) funds creative and innovative R&D projects at Argonne. Selection of projects is the responsibility of the laboratory director. The objectives of LDRD are to stimulate innovation and creativity, to continuously renew the scientific and technological vitality of the Laboratory, and to respond to rapidly emerging R&D opportunities. The program enhances Argonne's ability to attract and retain the high-caliber scientists and engineers essential for undertaking the Laboratory's missions for DOE and the nation. In addition, LDRD helps ensure that the Laboratory provides scientific and technical leadership in mission-related fields.

Argonne's primary project selection criteria are scientific and technical excellence, relationship to Laboratory strategic goals and objectives, innovativeness and cross-disciplinary character, expected contributions from the results, and prospects for continuation under programmatic support. Each year the laboratory director designates portions of the LDRD budget for support of particular types of projects. Categories include (1) competitive grants initiated by a principal investigator or a team on any mission-related topic and (2) projects directly related to the Laboratory's strategic initiatives. The immediate objectives of Argonne's LDRD portfolio are (1) to reinforce the Laboratory's R&D planning by supporting its mission and strategic view (as described in Chapter II of this *Institutional Plan)*, (2) to enrich the Laboratory's technical capabilities, (3) to encourage innovation and creativity by technical staff through the development of new concepts and principles and the undertaking of projects having high risk but potentially high reward, and (4) to exploit the Laboratory's technical potential for the benefit of the nation. In addition, the LDRD program has the very important outcome of enhancing the morale and vitality of the Laboratory's scientific and technical staff. Researchers' enthusiasm is nurtured by the knowledge that good new ideas, even those well beyond existing programs, are eligible to compete for the immediate funding they need.

Argonne's LDRD program supports promising novel and innovative projects wherever they may appear across the broad spectrum of science and technology relevant to current or prospective Laboratory missions. A report of accomplishments across the entire LDRD program is made to DOE each year. Some notable recent accomplishments include the following:

- Development of super-hard low-friction coatings for wear surfaces in diesel engines
- Design of high-throughput robotic devices for rapid characterization of biomolecular species
- Design of solid-state-based neutron detectors for survey and analysis of radiation fields produced by accelerators and other sources
- Ultra-miniaturization of multilayered ferroelectric capacitors for application to next-generation high-density data storage and nonvolatile memories
- Multivariate analysis of technical and economic factors affecting the transition from current-day power reactors to future-generation designs
- Development of a method based on gamma rays for the highly selective, highly sensitive detection of fissile materials
- Development and application of a scanning near-field magneto-optical microscope
- High-fidelity simulation of the human spine using parallel computing platforms
- Demonstration that direct etching with a focused-ion beam offers a feasible, possibly better method of fabricating high-resolution, high-efficiency microfocusing x-ray zone plates for use in scanning x-ray microprobes at synchrotron light sources

The larger component of LDRD emphasizes R&D aligned with Laboratory strategic initiatives, as reflected in this *Institutional Plan*. Strategic goals are periodically revised and reevaluated, as required. Existing staff expertise naturally causes a substantial number of employee-suggested LDRD projects to fall under the various high-priority initiative areas, so they can receive a correspondingly high priority in the proposal selection process. As discussed in Chapter III, current major Laboratory initiative areas include Nanosciences and Nanotechnology, the Rare Isotope Accelerator, Functional Genomics, Petaflops Computing and Computational Science, and Advanced Nuclear Fuel Cycle.

Several LDRD projects will be supported under the auspices of the Director's Competitive Grants component of the LDRD program. This component provides a direct avenue for single investigators and small multidisciplinary teams to propose projects to the laboratory director that do not fall within the Laboratory's defined strategic initiative areas, but that have high scientific or technical merit and are at the forefront of their fields. A Director's Review Committee, comprising scientists and engineers spanning the breadth of Argonne disciplines and programs, subjects Competitive Grants proposals to a thorough and highly competitive merit review. The resulting ranking is used by the laboratory director to select the winning proposals.

The LDRD program is funded Laboratory-wide through Argonne's indirect budget. As part of its LDRD planning before each fiscal year begins, the Laboratory proposes to DOE a maximum total LDRD expenditure. As indicated in Table IV.16, for FY 2002-FY 2004 this upper limit generally approximates 4.5% to 5.0% of projected total operating plus equipment funds for the Laboratory.

Table IV.16 Laboratory Directed R&D Funding ($ in millions)

	FY01[a]	FY02[b]	FY03[c]	FY04[c]
	20.9	20.9	21.5	22.5

[a] Actual expenditures.

[b] Authorized maximum expenditures for the LDRD program.

[c] Planned maximum expenditures for the LDRD program.